Approximated Solutions of Two-Point Nonlinear Boundary Problem by a Combination of Taylor Series Expansion and Newton Raphson Method

Chinwendu. B. Eleje, Udechukwu P. Egbuhuzor

***Abstract*—**One of the difficulties encountered in solving nonlinear Boundary Value Problems (BVP) by many researchers is finding approximated solutions with minimum deviations from the exact solutions without so much rigor and complications. In this paper, we propose an approach to solve a two point BVP which involves a combination of Taylor series expansion method and Newton Raphson method. Furthermore, the fourth and sixth order approximated solutions are obtained and we compare their relative error and rate of convergence to the exact solution. Finally, some numerical simulations are presented to show the behavior of the solution and its derivatives.

Keywords—Newton Raphson method, non-linear boundary value problem, Taylor series approximation, Michaelis-Menten equation.

I. Introduction

THE importance of enzymes in the management of life processes cannot be over emphasized. These enzymes are specific proteins stimulated by chemical reactions [1]. Based on some available data, enzymes can be used in diagnosing pathological disorders, drugs workability and disease treatment [2], [3]. These enzymatic reactions are seen to be very useful in the management of life processes and one of the equations arising from enzymatic reactions is a two point BVP known as the Michaelis-Menten equation. This Michaelis-Menten equation is a nonlinear linear differential equation and one of the most useful enzymatic kinetics models arising from the field of biochemistry and other related fields [4], [5]. This model is somehow difficult to solve for its exact solution due to its nonlinear nature. Hence, there is need to find a suitable numerical approach to solve this problem.

A lot of models derived in real life situations from different fields of mathematics and other related areas such engineering, biology, biochemistry, physics, biotechnology and even biomathematics often degenerate into linear or nonlinear differential equations. These equations may either be Ordinary Differential Equations (ODEs) or Partial Differential Equations (PDEs). The solutions of most linear ODEs and PDEs can be obtained by direct integration, separation of variable methods, Laplace transformation method, Fourier transformation method etc. [6]-[8]. However, most nonlinear differential equations be it ODEs or PDEs are not that easy to solve for their exact solutions. Hence, many researchers have developed different methods of solutions including analytical and numerical methods [9]-[19]. The numerical methods are used to obtain approximated solutions to any given problem. As often observed, most of these models are very difficult to solve for their exact solutions hence this has necessitated the use of approximated technique to obtain approximated solutions. Some of these methods include Adomian decomposition method [9], [10], differential transformation method [11], [12], the Taylor series approximation method [13], Fourier spectral method [14], Gamma function method [15], perturbation method [16], He frequency formulation and the dimensional method [17]-[19], homotopy perturbation method [20]-[26], the ancient Chinese algorithm [27] etc. These methods have been applied by many researchers in the field of medicine, biochemistry, pharmacy and biotechnology to solve enzymatic kinetics problems [28]. Specifically, the Michaelis-Menten equation has been solved for its approximated solutions using homotopy perturbation method [29], [30], Fourier spectral method [14], Ying Buzu algorithm [27], [31], [32] etc.

Also, another numerical method of solution used in solving differential equation is the Newton Raphson method. The method has been used by some researchers in [33]-[38]. Lately, the authors in [39] used a combination of Taylor series approximation and Ying Buzu algorithm to solve a two-point BVP for its fourth and sixth order solution. In this paper, we solve the Michaelis-Menten equation in [39] with modified boundary conditions using a combination of Taylor series approximation and Newton Raphson method to obtain the fourth and sixth order approximated solutions and compare the solution with [39] in terms of error and rate of convergence.

II. Kinetic Model

In this section, we introduce the kinematic model similar to the one in [1] and [39]. The following nonlinear BVP signify the law of mass action of oxygen:

$$\begin{cases} y''(x) = \frac{my(x)}{1+ny(x)}, \\ y(0) = mc, y(1) = 1 + c, y'(0) = 0 \end{cases} \quad (1)$$

where x is the dimension, m is the reaction diffusion parameter, y is the oxygen concentration and n the saturation parameter. Furthermore, we can rewrite (1) as:

Chinwendu. B. Eleje is with the Department of Computer Science and Informatic, Federal University Otuoke, Bayelsa State, Nigeria (e-mail: elejecb@fuotuoke.edu.ng).

Udechukwu P. Egbuhuzor is with the Department of Mathematics and Statistics, Federal University Otuoke, Bayelsa State, Nigeria.

$$\frac{d^2 y}{dx^2} + \mathcal{M}(y) = 0, \quad (2)$$

$$y'(a) = \alpha, \quad (3)$$

$$y(b) = \beta, \quad (4)$$

where y is a function of x, $y'(a) = \alpha$, $y(b) = \beta$ are the boundary conditions.

III. Methodology

A. The Newton Raphson Method

In this section, we discuss the Newton Raphson method. The method has been used by some researchers in [33]-[38] to solve some differential equations.

The Newton-Raphson method is a powerful tool for finding the root of an algebraic equation. It is an iterative method that uses initial values for the unknowns and then at each iteration, updates these values until no change occurs in two consecutive iterations. The Newton-Raphson formula is derived as follows: Let c_0 be an approximate value of a root of the equation $y(c) = 0$. Let c be the exact root nearer to c_0. Then

$$c = c_0 + h \quad (5)$$

where h is very small, positive or negative.

$$\therefore y(c) = y(c_0 + h) = 0$$

since c is the exact root of $y(c) = 0$. By Taylor expansion,

$$y(c) = y(c_0 + h) = \begin{pmatrix} y(c_0) + h y'(c_0) \\ + \frac{h^2}{2!} \ddot{y}(c_0) + \cdots \end{pmatrix} = 0 \quad (6)$$

Since h is small, $h^2, h^3, \ldots$ etc., are smaller. So, by neglecting terms with h^2, h^3, ...etc., we have

$$y(c_0) + h y'(c_0) = 0 \quad (7)$$

Solving for h in (7), we have

$$h = -\frac{y(c_0)}{y'(c_0)} \quad (8)$$

Substituting (7) in (5), we have $c = c_0 - \frac{y(c_0)}{y'(c_0)}$. In general,

$$c_{n+1} = c_n - \frac{y(c_n)}{y'(c_n)} \quad (9)$$

for $n = 0, 1, 2, 3$ ..., is the Newton-Raphson formula.

The condition for the validity of this formula and method is that $y(c_n) \neq 0$ and the condition for the convergence of the Newton-Raphson method is;

$$|v(x) v'(x)| < |v''(x)|^2$$

B. The Taylor Series Approximation Method

The Taylor series approximation for a second order nonlinear differential equation of the type similar to the one in [13], [27], is illustrated as follows: We consider the nonlinear BVP in (2)-(4) and if

$$y(c) = \alpha, \quad (10)$$

the infinite Taylor series expansion can be used to express the exact solution of (1).

From [13], [27], the Taylor series expansion for k^{th} order derivative is given as

$$\begin{cases} y(x) = y(c) + y'(c)(x-c) \\ + \frac{1}{2!} y''(c)(x-c)^2 + \frac{1}{3!} y'''(c)(x-c)^3 \\ + \cdots + \frac{1}{(k-1)!} y^{(k-1)}(c)(x-c)^{k-1} \\ + \frac{1}{k!} y^k(c)(x-c)^k \end{cases}, \quad (11)$$

where

$$\begin{cases} y(c) = \alpha, y'(c) = a, y''(c) = -K(\alpha), \\ y'''(c) = -a \frac{\partial K(\alpha)}{\partial v} \end{cases}$$

IV. Main Result

In this section, we will consider a typical kinetic model in (1) similar to [39], where $m = 2$, $n = 1$. The equation is given by (12):

$$y''(x) = \frac{2y(x)}{1 + y(x)}, \quad (12)$$

with boundary conditions of as

$$y(0) = 2c, \; y(1) = 1 + c, y'(0) = 0 \; . \quad (13)$$

From (12) and (13),

$$y''(0) = \frac{4c}{1+2c}, \quad (14)$$

$$y'''(0) = 0, \quad (15)$$

$$y^{iv}(0) = \frac{8c}{(1+2c)^3}, \quad (16)$$

$$y^{v}(0) = 0, \quad (17)$$

$$y^{vi}(0) = \frac{16c(1-12c)}{(1+2c)^5}. \quad (18)$$

A. The Fourth Order Solution

From (11), the fourth order Taylor series is given by

$$y(x) = y(0) + y'(0)x + \frac{1}{2!} y''(0)x^2 + \frac{1}{3!} y'''(0)x^3 + \frac{1}{4!} y^{iv}(0)x^4 \; . \quad (19)$$

Substituting (13)-(16) into (19), we will have

$$y(x) = 2c + \frac{2c}{1+2c} x^2 + \frac{c}{3(1+2c)^3} x^4 \; . \quad (20)$$

Substituting $y(1) = 1 + c$ into (20), we have $y(c) = c + \frac{2c}{1+2c} + \frac{c}{3(1+2c)^3} - 1$. Applying the Newton Raphson formula (9), we have $c_{n+1} = c_n - \frac{y(c_n)}{y'(c_n)}$ where

$$y(c_n) = c_n + \frac{2c_n}{1+2c_n} + \frac{c_n}{3(1+2c_n)^3} - 1 \,.$$
$$y'(c) = 1 + \frac{2}{(1+2c_n)^2} + \frac{1-4c_n}{3(1+2c_n)^4}$$

If we assume our initial guess to be $c_0 = 0.5$

$$y(c_0) = 0.02083, y'(c_0) = 1.47917$$
$$c_1 = c_0 - \frac{y(c_0)}{y'(c_0)} = 0.5 - \frac{0.02083}{1.47917} = 0.48592$$
$$\beta_1 = y(1, c_1) = 2c_1 + \frac{2c_1}{1+2c_1} + \frac{c_1}{3(1+2c_1)^3} = 1.48583 \,.$$

Next, we repeat the iteration till $c_n = c_{n+1}$, since $c_1 = 0.48592$,

$$y(c_1) = -0.000093996, \; y'(c_1) = 1.49358$$
$$c_2 = c_1 - \frac{y(c_1)}{y'(c_1)} = 0.48592 + \frac{0.000093996}{1.49358} = 0.48598$$
$$\beta_2 = y(1, c_2) = 2c_2 + \frac{2c_2}{1+2c_2} + \frac{c_2}{3(1+2c_2)^3} = 1.48598 \,.$$

Next, we repeat the iteration till $c_n = c_{n+1}$, since $c_2 = 0.48598$,

$$y(c_1) = -0.0000043834, \; y'(c_1) = 1.49351$$
$$c_3 = c_2 - \frac{y(c_2)}{y'(c_2)} = 0.48598 + \frac{0.0000043834}{1.49351} = 0.48598$$
$$\beta_3 = y(1, c_3) = 2c_3 + \frac{2c_3}{1+2c_3} + \frac{c_3}{3(1+2c_3)^3} = 1.48598 \,.$$

Since $c_2 = c_3$, we stop the iteration and we observed that the relative error is approximately zero. Hence, we obtain the fourth order approximated solution by substituting $c_3 = 0.48598$ into (20) as follows

$$y(x) = 0.97196 + 0.49289x^2 + 0.02113x^4 \,. \qquad (21)$$

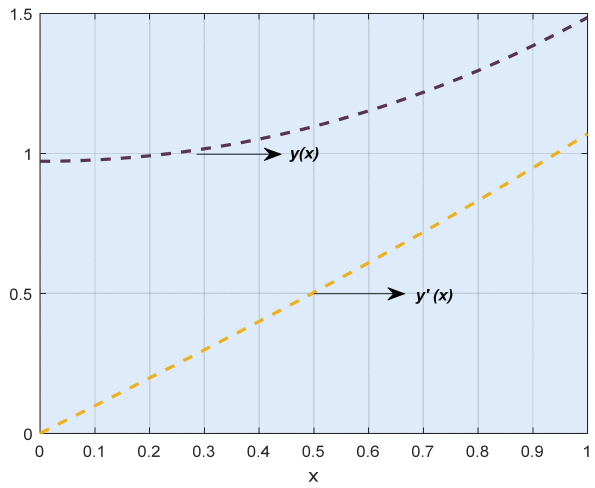

Fig. 1 The Fourth order solution

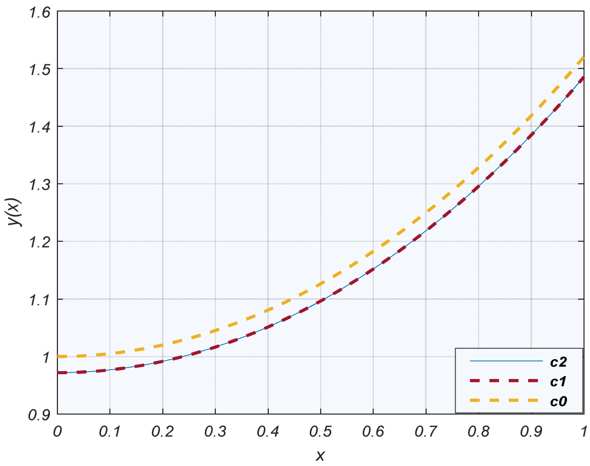

Fig. 2 The Fourth order solution with different initial guesses

B. The Sixth Order Solution

From (11), the fourth order Taylor series is given by

$$y(x) = y(0) + y'(0)x + \frac{1}{2!}y''(0)x^2 + \frac{1}{3!}y'''(0)x^3 + \frac{1}{4!}y^{iv}(0)x^4 + \frac{1}{5!}y^{v}(0)x^5 + \frac{1}{6!}y^{vi}(0)x^6 \,. \qquad (22)$$

Substituting (13)-(18) into (22), we will have

$$y(x) = 2c + \frac{2c}{1+2c}x^2 + \frac{c}{3(1+2c)^3}x^4 + \frac{c(1-12c)}{45(1+2c)^5}x^6 \,. \qquad (23)$$

Substituting $y(1) = 1 + c$ into (23), we have $y(c) = c + \frac{2c}{1+2c} + \frac{c}{3(1+2c)^3} + \frac{c(1-12c)}{45(1+2c)^5} - 1$. Applying the Newton Raphson formula (9), we have $c_{n+1} = c_n - \frac{y(c_n)}{y'(c_n)}$ where

$$y(c_n) = c_n + \frac{2c_n}{1+2c_n} + \frac{c_n}{3(1+2c_n)^3} + \frac{c_n(1-12c_n)}{45(1+2c_n)^5} - 1 \,.$$
$$y'(c) = 1 + \frac{2}{(1+2c_n)^2} + \frac{1-4c_n}{3(1+2c_n)^4} + \frac{48c_n^2 - 30c_n + 1}{45(1+2c_n)^6}$$

If we assume our initial guess to be $c_0 = 0.5$

$$y(c_0) = 0.0191, \; y'(c_0) = 1.47847$$
$$c_1 = c_0 - \frac{y(c_0)}{y'(c_0)} = 0.5 - \frac{0.0191}{1.47847} = 0.48708$$
$$\beta_1 = 2c_1 + \frac{2c_1}{1+2c_1} + \frac{c_1}{3(1+2c_1)^3} + \frac{c_n(1-12c_n)}{45(1+2c_n)^5} = 1.48697 \,.$$

Next we repeat the iteration till $c_n = c_{n+1}$ since $c_1 = 0.48708$,

$$y(c_1) = -0.00011105, \; y'(c_1) = 1.49153$$
$$c_2 = c_1 - \frac{y(c_1)}{y'(c_1)} = 0.48708 + \frac{0.00011105}{1.49153} = 0.48714$$
$$\beta_2 = 2c_2 + \frac{2c_2}{1+2c_2} + \frac{c_2}{3(1+2c_2)^3} + \frac{c_n(1-12c_n)}{45(1+2c_n)^5} = 1.48714 \,.$$

Since $c_2 = 0.48714$,

$$y(c_1) = -0.00001, \; y'(c_1) = 1.49146$$
$$c_3 = c_2 - \frac{y(c_2)}{y'(c_2)} = 0.48714 + \frac{0.00001}{1.49146} = 0.48714$$

$$\beta_3 = \mathcal{y}(1, c_3) = 2c_3 + \frac{2c_3}{1+2c_3} + \frac{c_3}{3(1+2c_3)^3} = 1.48714.$$

Since $c_2 = c_3$, we stop the iteration and we observed that the relative error is approximately zero. Hence, we obtain the sixth order approximated solution by substituting $c_3 = 0.48714$ into (23) as follows

$$\mathcal{y}(x) = 0.97428 + 0.49349x^2 + 0.02110x^4 - 0.0017488 \quad (24)$$

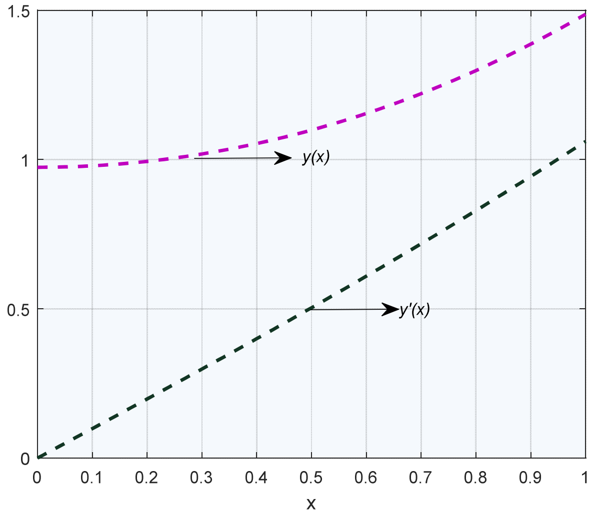

Fig. 3 The Sixth order solution

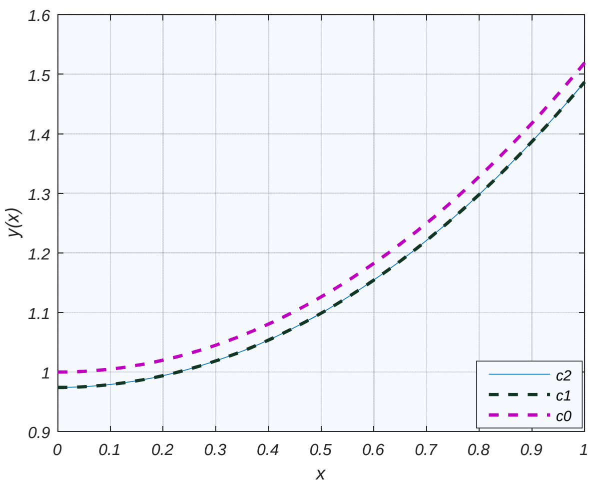

Fig. 4 The Sixth order solution with different initial guesses

V. Discussion and Conclusion

Fig. 1 shows the solution of the solution of the two-point BVP in (12) and the derivative of the solution. We observed that the solution was a curve while that of its derivative was a straight line. The graph also shows that the numerical solution satisfies the boundary conditions. We also observed that the fourth order solution obtained by the combination of Taylor series approximation and Newton Raphson method was similar to that obtained in [39] for the sixth order Ying Buzu Shu algorithm.

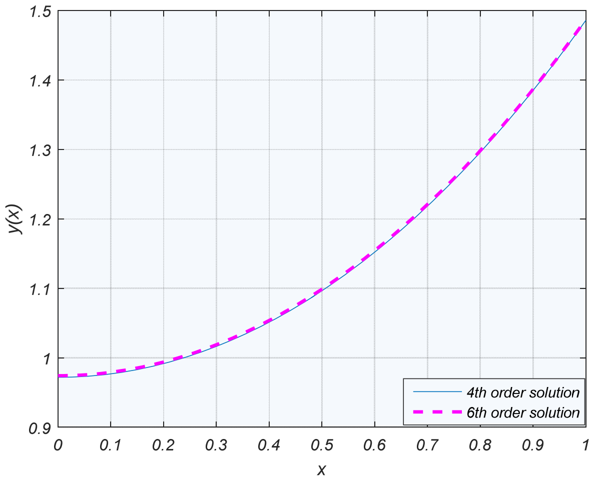

Fig. 5 Convergence of the fourth and sixth order solutions

Fig. 5 presents a comparison of the approximate solutions for the fourth and sixth order solution. It is observed that the fourth and sixth order approximate solutions converge very closely to the boundary conditions. Also, Figs. 2 and 4 show plots of the fourth and sixth order solution of the two-point BVP in (12) with different initial guesses. We observed that both c_1 and c_2 converge very closely to the exact solution.

In summary, the results obtained were very close to the results obtained in [39], secondly, the rate of convergence to solution is faster compared to Ying Buzu Shu algorithm with a small relative error. In conclusion, the combination of Taylor series approximation with Newton Raphson and a combination of Taylor with Ying Buzu Shu algorithm is more efficient than using Taylor series approximation only which is consistent with [27], [39]. Therefore, we conclude that solutions obtained with a combination of Taylor series with Newton Rapson method are more accurate than that of Taylor series approximation method solutions and the process is simple and straight forward.

References

[1] D. Omari, A. K. Alomari, A. Mansour A. Bawaneh, A, Mansour. Analytical Solution of the Non-linear Michaelis–Menten Pharmacokinetics Equation, Int. J. Appl. Comput. Math, (2020), 6-10. https://doi.org/10.1007/s40819-019-0761-5

[2] https://www.rosehulman.edu/~brandt/Chem330/Enzyme_kinetics.pdf

[3] B. Choi, G. Rempala, A., Kim, J. Kyoung. Beyond the Michaelis–Menten equation: accurate and efficient estimation of enzyme kinetic parameters. Sci. Rep. 7(2017), 17-26.

[4] Sun, He, Zhao, Hong: Chap 12: drug elimination and hepatic clearance. In: Chargel, L., Yu, A. (eds.) Edrs, Applied Biopharmaceutics and Pharmacokinetics, 7th edn, pp. 309–355. McGraw Hill, New York (2016)

[5] L. Rulí˘sek, S. Martin. Computer modeling (physical chemistry) of enzymecatalysis,metalloenzymes.https://www.uochb.cz/web/document/cms_library/2597

[6] T. G. Sudha, H. V. Geetha and S Harshini. solution of heat equation by method of separation of variable using the Foss tools maxima. International Journal of pure and applied mathematics, 117(12), (2017), 281-288.

[7] N. V. Vaidya, Deshpande, AA and Pidurkar, (2021). Solution of heat equation (Partial Differential Equation) by various methods S R Journal of Physics: Conference Series 1913 (2021) 012144 IOP Publishing doi:10.1088/1742-6596/1913/1/012144. 1-12.

[8] A. Abdulla – Al – Mamun, S Ali and M. MunnuMiah 2018 A study on

an analytic solution 1D heat equation of a parabolic partial differential equation and implement in computer programming, international Journal of Scientific & Engineering Research 9, Issue 9, 913 ISSN 2229-5518

[9] N. A. Udoh, U. P. Egbuhuzor, On the analysis of numerical methods for solving first order non linear ordinary differential equations. Asian Journal of Pure and Applied Mathematics, 4(3) (2022), 279-289.

[10] R. B. Ogunrinde, K. I Oshinubi. A Computational Approach to Logistic Model using Adomian Decomposition Method, Computing, Information System & Development Informatics Journal. 8(4) (2017). www.cisdijournal.org

[11] R. Bronson, G. Costa. Differential equations, third edition, Schaum's outline series. (2006). McGraw-Hill, New York.

[12] S. Momani, S. Abuasad, Z. Odibat. Variational iteration method for solving nonlinear boundary value problems. Applied Mathematics and Computation, 183(2006), 1351-1358.

[13] J. He. Taylor series solution for a third order boundary value problem arising in architectural engineering, Ain Shams Eng. J., 11 (2020), 1411–1414.

[14] C. Han, Y. Wang, Z. Li. Numerical solutions of space fractional variable-coefficient KdV modified KdV equation by Fourier spectral method, Fractals, (2021). https://doi.org/10.1142/S0218348X21502467.

[15] K. Wang, G. Wang. Gamma function method for the nonlinear cubic-quintic Du_ng oscillators, J. Low Freq. Noise V. A., (2021). https://doi.org/10.1177/14613484211044613.

[16] C. He, D. Tian, G. Moatimid, H. F. Salman, M. H. Zekry, Hybrid Rayleigh-Van der Pol Du_ng Oscillator (HRVD): Stability Analysis and Controller,

[17] D. Tian, Q. Ain, N. Anjum. Fractal N/MEMS: from pull-in instability to pull-in stability, Fractals, 29 (2021), 2150030.

[18] D. Tian, C. He, A fractal micro-electromechanical system and its pull-in stability, J. Low Freq. Noise V. A., 40 (2021), 1380–1386.

[19] C. He, S. Liu, C. Liu, H. Mohammad-Sedighi. A novel bond stress-slip model for 3-D printed concretes, Discrete and Continuous Dynamical System, (2021). http://dx.doi.org/10.3934/dcdss.2021161.

[20] Q.K Ghori, M. Ahmed, A. M. Siddiqui. Application of Homotopy perturbation method to squeezing flow of a Newtonian fluid, International Journal of Nonlinear Sciences and Numerical Simulation, 8 (2007), 179- 184. doi:10.1515/IJNSNS.2007.8.2.179

[21] T. Ozis, A. Yildirim. A comparative study of He's Homotopy perturbation method for determining frequency-amplitude relation of a nonlinear oscillator with discontinuities, International Journal of Nonlinear Sciences and Numerical Simulation, 8 (2007), 243-248. doi:10.1515/IJNSNS.2007.8.2.243

[22] S.J. Li, X.Y. Liu. An Improved approach to non-linear dynamical system identification using PID neural networks, International Journal of Nonlinear Sci- ences and Numerical Simulation, 7 (2006), 177-182. doi:10.1515/IJNSNS.2006.7.2.177

[23] M. M. Mousa, S.F Ragab, Z. Nturforsch. Application of the Homotopy perturbation method to linear and non-linear Schrödinger equations. Zeitschrift für Naturforschung, 63 (2008), 140-144.

[24] J.H. He. Homotopy perturbation technique. Com- puter Methods in Applied Mechanics and Engineering, 178 (1999), 257-262. doi:10.1016/S0045-7825(99)00018-3

[25] X. Li, C. He. Homotopy perturbation method coupled with the enhanced perturbation method, J. Low Freq. Noise V. A., 38 (2019), 1399–1403.

[26] U. Filobello-Nino, H. Vazquez-Leal, B. Palma-Grayeb. The study of heat transfer phenomena by using modified homotopy perturbation method coupled by Laplace transform, Thermal Science, 24 (2020), 1105–1115.

[27] J. He, S. Kou, H, Sedighi. An Ancient Chinese Algorithm for two point boundary problems and its application to the Michaelis-Menten Kinematics, Mathematical Modelling and Control, 1(4) (2021), 172-176.

[28] M. Golic. Exact and approximate solutions for the decades-old Michaelis–Menten equation: progress curve analysis through integrated rate equations. Biochem. Mol. Biol. Educ. 39(2) (2011), 117–125. https://doi.org/10.1002/bmb.20479

[29] D. Shanthi, V. Ananthaswamy, L. Rajendran. Analysis of non-linear reaction-diffusion processes with Michaelis-Menten kinetics by a new Homotopy perturbation method, Natural Science, 5(9) (2013), 1034-1046.http://dx.doi.org/10.4236/ns.2013.59128.

[30] D. Omari, A. K. Alomari, A. Mansour A. Bawaneh, A, Mansour. Analytical Solution of the Non-linear Michaelis–Menten Pharmacokinetics Equation, Int. J. Appl. Comput. Math, (2020), 6-10. https://doi.org/10.1007/s40819-019-0761-5

[31] C. He, A Simple Analytical Approach to a Non-Linear Equation Arising in Porous Catalyst, International Journal of Numerical Methods for Heat and Fluid-Flow, 27 (2017), 861–866.

[32] C. He, An Introduction an Ancient Chinese Algorithm and Its Modification, International Journal of Numerical Methods for Heat and Fluid-flow, 26 (2016), 2486–2491.

[33] J. F. Traup. Iterative methods for the solution of equations. Prentice, Englewood Cliffs, New Jer-sey (1964).

[34] J. M. Ortega and W. G. Rheinboldt Iterative Solution of Nonlinear Equations in Several Variables. Academic Press, New York. (1970)

[35] J. E Dennis and R. B. Schnabel Numerical methods for unconstrained optimization and nonlinear equations. SIAM, Philadelphia. (1993).

[36] C. T Kelley. Solving nonlinear equations with Newton's method. SIAM, Philadelphia. (2003).

[37] M. S. Petković, N. B, Petković and LD, Džunić Multipoint methods for solving nonlinear equations: a survy. Appl Mat Comput 226 (2013) 635–660

[38] J. R. Sharma, R. K Guha, R. Sharma. An efficient fourth order weighted-Newton method for systems of nonlinear equations. Numer Algorithms 62, (2013), 307–323.

[39] U. C. Amadi and N. A. Udoh Solution of two point boundary problem using Taylor series approximation and the Ying Buzu Shu algorithm, International Journal of mathematical and computational sciences, 16(8) (2022), 68–73.