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Numerical Solutions of Nonlinear Biochemical Model Using a Hybrid Numerical-Analytical Technique

S. O. Edeki [1*], E. A. Owoloko [1], A. S. Osheku [2], A. A. Opanuga [1], H. I. Okagbue [1] and G. O. Akinlabi[1]

[1]Department of Mathematical Sciences
Covenant University, Canaanland, Otta, Nigeria

[*]Corresponding author

[2] Department of Mathematics,
University of Ibadan, Ibadan, Nigeria

Abstract

In this paper, a hybrid numerical-analytical technique resulting from the combination of the differential transformation method and the Pade approximation technique; hereby referred to as differential transformation-Pade approximation technique (DTPAT) is introduced and applied for numerical solutions to the nonlinear biochemical reaction model. The obtained numerical results via the DTPAT are in excellent agreement with those obtained using ADM, PIM, RK4, HPM, and MPHM. The DTPAT increases the convergent rate of the series solutions obtained via the DTM, is showed to be very effective; it requires less computational work, and hence a promising technique for both linear and nonlinear systems in other areas of medical and biomedical sciences.

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Keywords: Biochemical reaction, Differential transform, Enzyme kinetic model, Nonlinear system, Pade' approximants

1 Introduction

The presence of enzymes being unique catalysts speeds up biochemical reactions immensely. This makes the kinetic of the concerned reaction different from that of the conventional chemical kinetics. In 1913, Michaelis and Menten [1] were the first to observe this, as they developed a quantitative theory for enzyme kinetics and as a result, they proposed a simple but powerful structural model in analyzing the enzyme processes [2, 3].
Thus, in consideration, we shall look at the basic Michaelis-Menten Enzyme Kinetic Model (MIC-MENEKM) resulting from the reaction scheme as follows [3, 4] as follows:

$$\xi + H \underset{\lambda^-}{\overset{\lambda^+}{\rightleftharpoons}} U \overset{\lambda^{++}}{\rightarrow} \xi + V \tag{1}$$

where ξ is the enzyme, H is the substrate, U is the enzyme-substrate complex, V is the product of H when metamorphosed, λ^+ is the first order rate constant, λ^{++} is the second order rate constant and λ^- is the first order rate for the reverse reaction.
Briggs and Haldane in [5] derived the Michaelis-Menten equation with a version in (1).
Based on the law of mass action, the rate of changes of the various species with respect to time t, leads to four differential equations:

$$\frac{dH}{dt} = -\lambda^+ \xi H + \lambda^- U \tag{2}$$

$$\frac{d\xi}{dt} = -\lambda^+ \xi H + cU \tag{3}$$

$$\frac{dU}{dt} = \lambda^+ \xi H - cU \tag{4}$$

$$\frac{dV}{dt} = \lambda^{++} U \tag{5}$$

where

$$c = \lambda^{-} + \lambda^{++} \tag{6}$$

with the initial conditions:

$$\xi(0) = \xi_0,\ H(0) = H_0,\ U(0) = U_0,\ \text{and } V(0) = V_0 \tag{7}$$

In dimensionless form of substrate concentration, m, and intermediate complex between ξ & H, n, equations (2)-(5) can be reduced to only two equations for H and U as given below; see [6] for more detail. Thus,

$$\eta \frac{dn}{dt} = m - \alpha n - mn \tag{8}$$

$$\frac{dm}{dt} = -m + (\alpha - \beta)n + mn \tag{9}$$

subject to:

$$m(0) = 1,\ n(0) = 0 \tag{10}$$

where the parameters b η, α and β are dimensionless.

In an attempt to solve the nonlinear system, Sen in [6] applied the ADM for an approximate analytical solution for the transient phase of the Michaelis-Menten reaction model. Khader introduced Picard-Pade technique (PPT) as a modification of Picard iteration method (PIM), he studied the convergence analysis of the proposed method, and tested its effectiveness using the basic enzyme kinetic model [7]. Batiha and Batiha in [8] applied the differential transformation method [DTM] to the MIC-MENEKM and confirmed the reliability and agreement of the method with the homotopy perturbation method (HPM).

Meanwhile, the DTM has been noted for both numerical and analytical solutions of differential equations [9-11]. Hashim *et al* converted the standard HPM into a hybrid method called the multistage HPM (MHPM), applied the result to the nonlinear biochemical reaction model (MIC-MENEKM), and confirmed that the numerical solutions are in excellent agreement with those from the classical fourth-order Runge-Kutta (RK4) method [12]. The DTM has a wider range of applications in dealing with models involving integro-differential equations in finance and actuarial sciences [13].

In this work, we present a hybrid numerical-analytical method (DTPAT) resulting from the modification of the DTM based on Pade approximation. For effectiveness and reliability, the method is applied to the MIC-MENEKM, and the numerical results obtained are compared with those from other standard methods.

2 The Basic Models

This section takes care of the basic models used in this paper.

2.1 *The Differential Transform Method (DTM)*

This subsection introduces the basic concepts and theorems of DTM needed for applications in the remaining sections.

Definition 1. Let $w(x)$ be a given function of one variabe defined at a point $x = x_0$, then the one-dimensional k^{th} differential transform of $w(x)$ defined as $W(k)$ is:

$$W(k) = \frac{1}{k!}\left(\frac{d^k w(x)}{dx^k}\right)\Bigg|_{x=x_0} \tag{11}$$

Definition 2. The inverse differential transform of $W(k)$ is a Taylor series expansion of the function $w(x)$ about $x = x_0 = 0$, defined as :

$$w(x) = \sum_{k=0}^{\infty} W(k)x^k \tag{12}$$

Combining (11) and (12) yields:

$$w(x) = \sum_{k=0}^{\infty}\left(\frac{d^k w(x)}{dx^k}\right)\frac{x^k}{k!} \tag{13}$$

2.2 *Some Basic Theorems of the Differential Transform Method*

The following theorems and properties of the DTM are stated below for the issues of applications while their proofs and further properties can be found in standard numerical texts and referred journals: see [14,15] and the references therein.

Let $w_1(x)$, $w_2(x)$ and $w_*(x)$ be differentiable functions with differential transforms $W_1(k)$, $W_2(k)$ and $W_*(k)$ respectively, with $n \geq 0$, $\alpha_i \in \mathbb{R}$ and δ a kronecker delta, then the following theorems hold:

Theorem 1 If $y = \alpha_1 w_1(x) \pm \alpha_2 w_2(x)$ then $Y(k) = \alpha_1 W_1(k) \pm \alpha_2 W_2(k)$

Theorem 2 If $y = x^n$ then $Y(k) = \delta(\mathrm{k-n})$ such that:

$$Y(k) = \delta(\mathrm{k-n}) = \begin{cases} 1, & k=n \\ 0, & \text{otherwise} \end{cases}$$

Theorem 3 If $y = w_1(x) w_2(x)$, then $Y(k) = \sum_{\tau=0}^{k} W_1(\tau) W_2(k-\tau)$

Theorem 4 If $y = \frac{d^n}{dx^n}\left[w_*(x)\right]$, then $Y(k) = \frac{(k+n)!}{n!} W_*(k+n)$.

In particular, we have:

* If $y = \frac{d}{dx}\left[w_*(x)\right]$, then $Y(k) = (k+1) W_*(k+1)$

2.3 *Pade Approximant of a Power Series Solution*

Most solutions of differential equations- ordinary or partial follow power series forms; these solutions become numerical solutions of the associated differential equations upon approximation or truncation.

These power series are often approximated by polynomials, nevertheless, polynomials tend to exhibit oscillations that may produce error bounds, also, the singularities of polynomials cannot be observed clearly in a finite plane [16, 17]; hence, the transformation of the power series for numerical approximation using Pade approximants.

A Pade approximant of a function is a rational function of two polynomial functions where the coefficients of the numerator and the denominator depend on the coefficients of the concerned function [17-19]. Thus, the following definitions:

Definition 3: Let $g(x)$ be a function defined on the interval $I = [a, \mathrm{b}]$, with a Taylor series expansion $\sum_{i=0}^{\infty} k_i x^i$, such that

$$g(x) = \sum_{i=0}^{\infty} k_i x^i, k \geq 0 \tag{14}$$

Suppose

$$g(x)=\frac{A_0+A_1x+A_2x^2+\cdots A_{\wp}x^{\wp}+\cdots}{B_0+B_1x+B_2x^2+\cdots+B_{\Im}x^{\Im}+\cdots}=\frac{\sum_{i=0}^{\infty}A_jx^j}{\sum_{i=0}^{\infty}B_ix^i} \tag{15}$$

Then, the Pade Approximant of $g(x)$ is defined as:

$$P_{\{g(x)\}}\left[\wp\middle|\Im\right]=\frac{\sum_{j=0}^{\wp}A_jx^j}{\sum_{i=0}^{\Im}B_ix^i}=\frac{Q_{\wp}(x)}{Q_{\Im}^{*}(x)} \tag{16}$$

where $Q_{\wp}(x)$ and $Q_{\Im}^{*}(x)$ are polynomials of degree $\wp$ and $\Im$ respectively.

Remark 1: For the avoidance of a common factor in (16), we shall set $B_0=1$, as such, (16) is expressed as:

$$P_{\{g(x)\}}\left[\wp\middle|\Im\right]=\frac{A_0+A_1x+A_2x^2+\cdots A_{\wp}x^{\wp}}{1+B_1x+B_2x^2+\cdots+B_{\Im}x^{\Im}} \tag{17}$$

It can be seen from (17) that the numerator and the denominator contain $(1+\wp)$ and $(\Im)$ coefficients respectively; hence, in computing $[\wp|\Im]$, a total of $(1+\wp+\Im)$ coefficients are to be determined.

Definition 4: Diagonal Approximant

The Pade approximant in (16)-(17) is said to be a diagonal approximant if the numerator and the denominator are of the same degree (i.e. $\wp=\Im$). In what follows, we shall be using the diagonal approximants for more accuracy and efficiency.

3. Applications and the Basic Methodology

3.1 *The DTPAT applied to MIC-MENEKM*

In this subsection, the DTM will be applied to the system of differential equations in (8) and (9) to obtain n and m, and thereafter, the computation of the Pade approximants for interpretation. Thus, (8) and (9) becomes:

$$\eta(k+1)N(k+1) = M(k) - \alpha N(k) - \sum_{r=0}^{k} M(r)N(k-r) \tag{18}$$

and

$$(k+1)M(k+1) = -M(k) + (\alpha - \beta)N(k) + \sum_{r=0}^{k} M(r)N(k-r) \tag{19}$$

subject to

$$M(0) = 1 \text{ and } N(0) = 0 \tag{20}$$

resulting from the initials $m(0) = 1$ and $n(0) = 0$.
For simplicity and ease of calculation, we re-write the recurrence relations (18) and (19) as:

$$N(k+1) = \frac{1}{\eta(k+1)}\left\{M(k) - \alpha N(k) - \sum_{r=0}^{k} M(r)N(k-r)\right\} \tag{21}$$

and

$$M(k+1) = \frac{1}{k+1}\left\{-M(k) + (\alpha - \beta)N(k) + \sum_{r=0}^{k} M(r)N(k-r)\right\} \tag{22}$$

with the same initial conditions as in (20).
For numerical computation and comparison, the case when $\alpha = 1.0$, $\beta = 3/8$ and $\eta = 1/10$ will be considered. Therefore, using (20),(21) and (22), we have:

for $k = 0,\ N(1) = 10,$ and $M(1) = -1$,

for $k = 1,\ N(2) = -105,$ and $M(2) = 69/8$,

for $k = 2,\ N(3) = 9145/12,$ and $M(3) = -757/12$,

for $k = 3,\ N(4) = -17785/4,$ and $M(4) = 47767/128$,

for $k = 4,\ N(5) = 4440661/192,$ and $M(5) = -3800401/1920$,

for $k = 5,\ N(6) = -44551057/384,$ and $M(6) = 156000923/15360$,

and so on for $k \geq 6$. Whence, using the computed coefficients, we have that:

$$\begin{aligned} n(t) &= \sum_{k=0}^{\infty} N(k)t^k \\ &= 10t - 105t^2 + \frac{9145}{12}t^3 - \frac{17785}{4}t^4 + \frac{4440661}{192}t^5 - \frac{44551057}{384}t^6 + \cdots \end{aligned} \tag{23}$$

and

$$\begin{aligned} m(t) &= \sum_{k=0}^{\infty} M(k)t^k \\ &= 1 - t + \frac{69}{8}t^2 - \frac{757}{12}t^3 + \frac{47767}{128}t^4 - \frac{3800401}{1920}t^5 + \frac{156000923}{15360}t^6 + \cdots \end{aligned} \tag{24}$$

For simplicity and ease of computation with regard to Pade approximant, we write the following in decimal forms:

$$n(t) = 10t - 105t^2 + 762\cdot0t^3 - 4446\cdot3t^4 + 23128\cdot4t^5 - 116018\cdot4t^6 + \cdots \tag{25}$$

and

$$m(t) = 1 - t + 8\cdot625t^2 - 63\cdot1t^3 + 373\cdot2t^4 - 1979\cdot4t^5 + 10156\cdot3t^6 + \cdots \tag{26}$$

3.2 *The Differential Transform-Pade Approximant Technique (DTPAT)*

The next task is to find the Pade approximant of the results in (25) and (26) obtained using the differential transform technique. To do this, we invoke (17) and consider a case when $\wp = \Im = 3$, thus, (25) and (26) become:

$$n(t) = \sum_{k=0}^{6} N(k)t^k = \frac{\sum_{j=0}^{3} A_j t^j}{\sum_{i=0}^{3} B_i t^i} = P_{\{n(t)\}}\left[3 \middle| 3\right], \text{ with } B_0 = 1 \tag{27}$$

and

$$m(t) = \sum_{k=0}^{6} M(k)t^k = \frac{\sum_{j=0}^{3} C_j t^j}{\sum_{i=0}^{3} D_i t^i} = P_{\{m(t)\}}\left[3 \middle| 3\right], \text{ with } D_0 = 1 \tag{28}$$

Thus,

$$P_{\{n(t)\}}\left[3\middle|3\right]=\frac{A_0+A_1t+A_2t^2+A_3t^3}{1+B_1t+B_2t^2+B_3t^3}=10t-105t^2+762\cdot 0t^3-4446\cdot 3t^4$$
$$+23128\cdot 4t^5-116018\cdot 4t^6$$

$\Rightarrow$

$$\begin{aligned}A_0+A_1t+A_2t^2+A_3t^3=\Big[&0+10t+(-105+10B_1)t^2+(762-105B_1+10B_2)t^3\\&+(-4446\cdot 3+762B_1-105B_2+10B_3)t^4\\&+(23128\cdot 4-4446\cdot 3B_1+762B_2-105B_3)t^5\\&+(-116018\cdot 4+23128\cdot 4B_1-4446\cdot 3B_2+762B_3)t^6\Big]\end{aligned}$$

So, for comparison of coefficients:

$$t^6:\ -116018\cdot 4+23128\cdot 4B_1-4446\cdot 3B_2+762B_3=0 \tag{29}$$

$$t^5:\ 23128\cdot 4-4446\cdot 3B_1+762B_2-105B_3=0 \tag{30}$$

$$t^4:\ -4446\cdot 3+762B_1-105B_2+10B_3=0 \tag{31}$$

$$t^3:\ 762-105B_1+10B_2=A_3 \tag{32}$$

$$t^2:\ -105+10B_1=A_2 \tag{33}$$

$$t^1:\ 10=A_1 \tag{34}$$

$$t^0:\ 0=A_0 \tag{35}$$

Solving the above system of linear equations simultaneously yields the following:

$$A_0=0,\ A_1=10,\ A_2=1\cdot 471549,\ A_3=63\cdot 71662,\ B_0=1,$$
$$B_1=10\cdot 64715,\ B_2=41\cdot 9669,\ \text{and } B_3=73\cdot 96808$$

Therefore,

$$P_{\{n(t)\}}\left[3\middle|3\right]=\frac{\sum_{j=0}^{3}A_jt^j}{\sum_{i=0}^{3}B_it^i}=\frac{10t+1\cdot 471549t^2+63\cdot 71662t^3}{1+10\cdot 64715t+41\cdot 96679t^2+73\cdot 96808t^3} \tag{36}$$

Similarly, for (19):

$$P_{\{m(t)\}}\left[3\middle|3\right]=\frac{C_0+C_1t+C_2t^2+C_3t^3}{1+D_1t+D_2t^2+D_3t^3}$$
$$=1-t+8\cdot 625t^2-63\cdot 1t^3+373\cdot 2t^4-1979\cdot 4t^5+10156\cdot 3t^6$$

$\Rightarrow$

$$\begin{aligned}C_0+C_1t+C_2t^2+C_3t^3\equiv\big[&1+(-1+D_1)t+(8\cdot 625-D_1+D_2)t^2\\&+(-63\cdot 1+8\cdot 625D_1-D_2)t^3\\&+(373\cdot 2-63\cdot 1D_1+8\cdot 625D_2-D_3)t^4\\&+(-1979.4+373\cdot 2D_1-63\cdot 1D_2+8\cdot 625D_3)t^5\\&+(10156\cdot 3-1979\cdot 4D_1+373\cdot 2D_2-63\cdot 1D_3)t^6\big]\end{aligned}$$

So, by equating the coefficients, we have:

$$t^6:\ 10156\cdot 3-1979\cdot 4D_1+373\cdot 2D_2-63\cdot 1D_3=0 \tag{37}$$

$$t^5:\ -1979\cdot 4+373\cdot 2D_1-63\cdot 1D_2+8\cdot 625D_3=0 \tag{38}$$

$$t^4:\ 373\cdot 2-63\cdot 1D_1+8\cdot 625D_2-D_3=0 \tag{39}$$

$$t^3:\ -63\cdot 1+8\cdot 625D_1-D_2=C_3 \tag{40}$$

$$t^2:\ 8\cdot 625-D_1+D_2=C_2 \tag{41}$$

$$t^1:\ -1+D_1=C_1 \tag{42}$$

$$t^0:\ 1=C_0 \tag{43}$$

Solving the above system of linear equations simultaneously gives:

$$C_0=1,\ C_1=8\cdot 143324,\ C_2=28\cdot 21359,\ C_3=-12\cdot 9707,$$
$$D_0=1,\ D_1=9\cdot 143324,\ D_2=28\cdot 73191,\ \text{and } D_3=44\cdot 069$$

Thus,

$$P_{\{m(t)\}}\left[3\middle|3\right]=\frac{\sum_{i=0}^{3}C_it^i}{\sum_{i=0}^{3}D_it^i}=\frac{1+8\cdot 143324t+28\cdot 21359t^2-12\cdot 9707t^3}{1+9\cdot 143324t+28\cdot 73191t^2+44\cdot 069t^3} \tag{44}$$

It is obvious from (22) and (23) that $\lim_{t\to\infty} P_{\{n(t)\}}[3|3] \in [-1,1]$ and $\lim_{t\to\infty} P_{\{m(t)\}}[3|3] \in [-1,1]$ since Pade approximants fluctuate between the interval $I = [-1,1]$ whenever the dependent variable tends to infinity [16].

4. Discussion of Results

In this subsection, we shall compare our result with those obtained using other numerical methods. As such, the results of the: DTM in (25) and (26), HPM & MHPM in [12], and DTPAT in (36) and (44) will be discussed as follows:

Table 1: for the solutions of the systems

Time t	$n(t)$:DTM 6-iterate	$P_{\{n(t)\}}\left[3\middle|3\right]$	$m(t)$: DTM 6-iterate	$P_{\{m(t)\}}\left[3\middle|3\right]$
0.0	0.0000	0.000000	1.000000	1.000000
0.1	0.71200	0.421534	0.950832	0.927764
0.2	3.89600	0.475679	1.253915	0.843655
0.3	14.1240	0.486822	5.389471	0.749064
0.4	35.9680	0.497580	28.82667	0.657679
0.5	74.0000	0.511581	114.9297	0.575128
0.6	132.792	0.527443	358.1763	0.502544
0.7	216.916	0.543796	934.6891	0.439300
0.8	330.944	0.559808	2140.079	0.384245
0.9	479.448	0.575049	4434.601	0.336175
1.0	667.000	0.589332	8495.625	0.294007

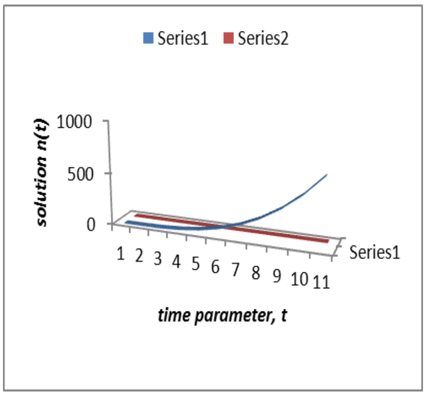

Figure 1: Solution for *n(t):* DTM 6-iterate (Series 1) & $P_{\{n(t)\}}\left[3\middle|3\right]$ (Series 2)

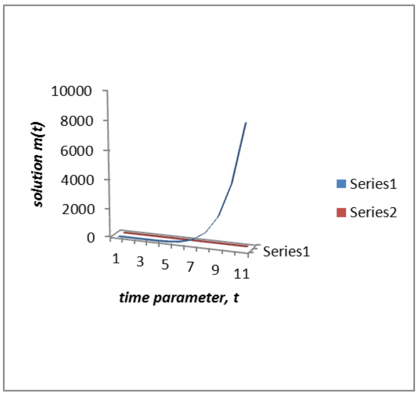

Figure 2: Solution for *m(t):* DTM 6- iterate (Series1) & $P_{\{n(t)\}}\left[3\middle|3\right]$ (Series 2)

Concluding Remarks

In this paper, we have introduced a hybrid numerical-analytical method (DTPAT), and applied it to a nonlinear biochemical reaction model (MICMENEKM). The numerical solutions obtained are in conformance with those obtained using the ADM, PIM, RK4, HPM, and MPHM. The DTPAT is very reliable and consistence even in a longer time frame and in a bigger interval; hence, a promising technique for both linear and nonlinear differential systems.

Conflict of Interests

The authors declare that there is no existence of conflict of interest.

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