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An Application of the Homotopy Analysis Method to the Transient Behavior of a Biochemical Reaction Model

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Abstract: In this paper, the homotopy analysis method (HAM) is applied to solve fractional transient phase of the Michaelis-Menten reaction. The analytical solution, which is given in the form of a power series, is found to be highly accurate in predicting the behavior of the reaction in the very early stages. The fractional derivatives are described by Caputo's sense. We also present a comparison of the various analytical approximations and a direct numerical solution of this problem. The results of applying this procedure to the studied cases show the high accuracy and efficiency of the approach.

Keywords: Homotopy Analysis Method, Fractional Calculus, Michaelis-Menten Biochemical Reaction Model

1 Introduction

Mathematical models based on ordinary differential equations appear in the real applications especially in biology because many biological laws and relations appear mathematically in the form of ordinary differential equations. Such models help to understand the underlying principles biological phenomena [1-10]. Here we propose the use of fractional calculus, because of the fact that the realistic modeling of a natural phenomenon does not depend only on the instant time, but also on the history of the previous time which can be successfully achieved by using fractional calculus. In other words, fractional order ordinary differential equations (FODEs) are that they are naturally related to systems with memory which exists in most biological systems. Main claim is that a fractional model can give a more realistic interpretation of natural phenomena. However, numerical methods commonly need large computation work and have round-off error problems. The Homotopy Analysis Method (HAM) which first proposed in 1992 by liao [11] is successful method to find the exact analytical solutions for linear and nonlinear problem. This method has been successfully applied into physics, chemical, biology, engineering fields and science [12-16]. In this paper, we present a solution of a more general model of an enzyme-catalyzed reaction model:

$$D_t^{\alpha_1} a = -a + (\beta - \alpha) y + a y,$$
$$D_t^{\alpha_2} y = \frac{1}{\varepsilon}(a - \beta y - a y) \qquad (1)$$

Subject to the initial conditions

$$a(0) = 1, y(0) = 0 \qquad (2)$$

Where a is a concentrations of substrate, y is an intermediate complex between enzyme and α, β, ε are dimensionless parameters. For more details of the standard model see [17-18].

2 Basic definitions

In this section, we mention the basic definitions of the fractional calculus.

Definition 1 The Riemann-Liouvlle fractional integral operator (J^{α}) of order$\alpha \geq 0$,
of a function $h \in c_{\mu}$,$\mu \geq -1$ Is defined as;

$$J^{\alpha} h(t) = \frac{1}{\Gamma(\alpha)} \int_0^t (t-\tau)^{\alpha-1} h(\tau) d\tau \quad (\alpha \succ 0)$$

$$J^0 h(t) = h(t)$$

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$\Gamma(\alpha)$ is the well-known gamma function some of the properties of the operator(J^{α}), Which we will need here, are as follows. for $h \in c_{\mu}$,$\mu \geq -1,\alpha,\beta \geq 0$ and $\gamma \geq -1$:

$$(1) J^{\alpha}J^{\beta}h(t) = J^{\alpha+\beta}h(t),$$

$$(2)\ J^{\alpha}J^{\beta}h(t) = J^{\beta}J^{\alpha}h(t),$$

$$(3)\ J^{\alpha}t^{\gamma} = \frac{\Gamma(\gamma+1)}{\Gamma(\gamma+\alpha+1)}t^{\alpha+\gamma}$$

$$J^{\alpha}e^{at} = t^{\alpha}\sum_{k=0}^{\infty}\frac{(at)^k}{\Gamma(\alpha+k+1)}$$

Definition 2 The fractional derivative of f(x) in the Caputo sense is defined as:

$$D^{\alpha}f(x) = J^{n-\alpha}D^n f(x) = \frac{1}{\Gamma(n-\alpha)}\int_0^x (x-t)^{n-\alpha-1}f^{(n)}(t)\,dt,$$

For $n-1<\alpha<n$,$n \in N$, x >0 .for the Caputo derivative we have$D^{\alpha}C = 0$, C is constant and

$$D^{\alpha}t^m == \begin{cases} 0 & m \leq \alpha-1 \\ \frac{\Gamma(m+1)}{\Gamma(m-\alpha+1)}\ , & m > \alpha-1 \end{cases}$$

Definition 3 For n to be the smallest integer that exceeds α, the Caputo fractional derivatives of order $\alpha>0$ is defined as

$$D^{\alpha}u(x,t) = \frac{\partial^{\alpha}u(x,t)}{\partial t^{\alpha}} = \begin{cases} \frac{1}{\Gamma(n-\alpha)}\int_0^t (t-\tau)^{n-\alpha+1}\frac{\partial^{\alpha}u(x,\tau)}{\partial\tau^{\alpha}}\,d\tau, & for\ n-1<\alpha\leq n, \\ \frac{\partial^n u(x,t)}{\partial t^{\alpha}}, & for\,\alpha=n \in N. \end{cases}$$

3 Homotopy analysis method

Let us consider the following system of differential equation

$$N_i[u_1(r,t),...,u_n(r,t)] = 0, i = 1,2,3,\ldots,n. \qquad (3)$$

Subject to the following initial conditions:

$$u_k(r,t) = c_k, k = 1,2,3,...,n. \qquad (4)$$

where N_i nonlinear operators that represent the whole equations, r and t are denote the independent variables and $u_i(r,t)$are unknowns function respectively. By means of generalizing the traditional homotopy method, Liao [11] constructed the so-called zero-order deformation equations for i=1, 2, . . . , n,

$$(1-q)\varphi_i[\phi_i(r,t;q)-u_{i0}(r,t)] = qh_iH_i(r,t)N_i[\phi_1(r,t;q),...,\phi_n(r,t;q)], \qquad (5)$$

where q∈[0,1] is the embedding parameter,$h_i \neq 0$ are non-zero auxiliary parameters for$H_i(r,t) \neq 0$ are non-zero auxiliary functions,$\varphi_i = D_t^{\alpha_i}(n-1<\alpha\leq n)$ are auxiliary linear operator with the following property for i=1,2,3,...,n

$$\varphi_i[\phi_i(r,t)] = 0 when \phi_i(r,t) = 0 \qquad (6)$$

$u_{i0}(r,t)$are initial guess of $u_i(r,t)$, $u_i(r,t;q)$are unknown function, respectively. It is important, that one has great freedom to choose auxiliary things in HAM. Obviously, when q=0 and q=1, it holds

$$\phi_i(r,t;0) = u_{i0}(r,t), \phi_i(r,t;1) = u_i(r,t), i = 1,2,...,n, \quad (7)$$

respectively. Thus, as q increases from 0 to 1, the solution $\phi_i(r,t,q)$varies from the initial guesses$u_{i0}(r,t,)$to the solution$u_i(r,t,)$. Expanding $\phi_i(r,t,q)$in Taylor series with respect to q, we have

$$\phi_i(r,t,q) = u_{i0}(r,t) + \sum_{m=1}^{+\infty}u_{im}(r,t)q^m, i = 1,2,\ldots,n. \quad (8)$$

where

$$u_{im}(r,t) = \frac{1}{m!}\left.\frac{\partial^m\phi_i(r,t;q)}{\partial q^m}\right|_{q=0}, i = 1,2,\ldots,n. \qquad (9)$$

If the auxiliary linear operator, the initial guess, the auxiliary parameter h, and the auxiliary function are so properly chosen, the series Eq. (16) converges at q= 1, then we have

$$\phi_i(r,t,q) = u_{i0}(r,t) + \sum_{m=1}^{+\infty}u_{im}(r,t), i = 1,2,\ldots,n. \quad (10)$$

Define the vector $\vec{u}_n^{\,i} = \{u_{i0}(r,t),u_{i1}(r,t),u_{i2}(r,t),...,u_{in}(r,t)\}$, i=1, 2, ..., n, Differentiating Eq. (13) times with respect to the embedding parameter q and then setting q=0 and finally dividing them by m!, we obtain the mth-order deformation equation for i =1,2,. . . ,n,

$$\varphi_i[u_{im}(r,t)-u_{im-1}(r,t)] = h_iH_i(r,t)R_{im}(\vec{u}_{m-1}^{\,1}(r,t),...,\vec{u}_{m-1}^{\,1}(r,t)) \qquad (11)$$

where

$$R_{im}(\vec{u}_{m-1}^{\,1}(r,t),...,\vec{u}_{m-1}^{\,n}(r,t)), \\ = \frac{1}{(m-1)!}\left.\frac{\partial^{m-1}N_i[\phi_1(r,t;q),...,\phi_n(r,t;q)]}{\partial q^{m-1}}\right|_{q=0} \qquad (12)$$

And

$$\chi_m = \begin{cases} 0 & m\leq 1, \\ 1 & m>1. \end{cases} \qquad (13)$$

Applying the Riemann–Liouville integral operator J^{α_i}on both side of Eq. (19), we have

$$u_{im} = \chi_m u_{im-1} + h_iH_i(r,t)J^{\alpha_i}[R_{im}(\vec{u}_{i\,m-1}(r,t),...,\vec{u}_{m-1}^{\,i}(r,t))]. \qquad (14)$$

In this way, it is easily to obtain $u_{i,m}(r,t)$ for$m \geq 1$, at Mth order, we have

$$u_i(r,t) = \sum_{m=0}^{\infty}u_{im}(r,t), i = 1,2,3,\ldots,n. \qquad (15)$$

We get an accurate approximation of the original Eq.(11).

4 Applications of the HAM

In this section, we apply the homotopy analysis method to solve the system

$$D_t^{\alpha_1} a = -a + (\beta - \alpha) y + ay,$$

$$D_t^{\alpha_2} y = \frac{1}{\varepsilon} (a - \beta y - ay), \tag{16}$$

Subject to the initial conditions

$$a(0) = 1, \ y(0) = 0. \tag{17}$$

We choose the linear operator

$$\begin{aligned} L_1 [\phi(x,y,t;q)] &= D_t^{\alpha_1} \phi(x,y,t;q) \quad , \quad L_1^{-1} = J^{\alpha_1} \phi(x,y,t;q) \\ L_2 [\phi(x,y,t;q)] &= D_t^{\alpha_2} \phi(x,y,t;q) \quad , \quad L_2^{-1} = J^{\alpha_2} \phi(x,y,t;q) \end{aligned} \tag{18}$$

With the property $L_1[c] = L_2[c] = 0$, where c is constant. We now define a nonlinear operator as:

$$\begin{aligned} N_1[\phi_1(x,y,t;q)] &= D_t^{\alpha_1} \phi_1(x,y,t) + \phi_1(x,y,t) - (\beta - \alpha)\phi_2(x,y,t) - \phi_1(x,y,t)\phi_2(x,y,t), \\ N_2[\phi_2(x,y,t;q)] &= D_t^{\alpha_2} \phi_2(x,y,t) - \tfrac{1}{\varepsilon}\phi_1(x,y,t) + \tfrac{\beta}{\varepsilon}\phi_2(x,y,t) + \tfrac{1}{\varepsilon}\phi_1(x,y,t)\phi_2(x,y,t) \end{aligned} \tag{19}$$

Using above definition, with assumption H (τ) =1 we construct the zero order deformation equation

$$\begin{aligned} (1-q)L_1 [\phi_1(x,y,t;q) - a_0(x,y,t)] &= qhN_1[\phi_1(x,y,t;q)], \\ (1-q)L_2 [\phi_2(x,y,t;q) - y_0(x,y,t)] &= qhN_2[\phi_2(x,y,t;q)] \end{aligned} \tag{20}$$

Obviously, when q=0and q=1,

$$\begin{aligned} \phi_1(x,y,t;0) &= a_0(x,y,t) \quad , \quad \phi_1(x,y,t;1) = a(x,y,t) \\ \phi_2(x,y,t;0) &= y_0(x,y,t) \quad , \quad \phi_2(x,y,t;1) = y(x,y,t) \end{aligned} \tag{21}$$

Thus, we obtain the mth–order deformation equations

$$\begin{aligned} L_1[a_m - \chi_m a_{m-1}] &= hR_m(\vec{a}_{m-1}), \\ L_2[y_m - \chi_m y_{m-1}] &= hR_m(\vec{y}_{m-1}) \end{aligned} \tag{22}$$

where

$$\begin{aligned} R_m(\vec{a}_{m-1}) &= D_t^{\alpha_1} a_{m-1} + a_{m-1} - (\beta - \alpha) y_{m-1} - \textstyle\sum_{i=0}^{m-1} a_i y_{m-1-i}, \\ R_m(\vec{y}_{m-1}) &= D_t^{\alpha_2} y_{m-1} - \tfrac{1}{\varepsilon} a_{m-1} + \tfrac{\beta}{\varepsilon} y_{m-1} + \tfrac{1}{\varepsilon} \textstyle\sum_{i=0}^{m-1} a_i y_{m-1-i} \end{aligned} \tag{23}$$

Now, the solution of the mth-order deformation equation (23)

$$\begin{aligned} a_m &= \chi_m a_{m-1} + hJ^{\alpha_1}[R_m(\vec{a}_{m-1})], \\ y_m &= \chi_m y_{m-1} + hJ^{\alpha_2}[R_m(\vec{y}_{m-1})] \end{aligned} \tag{24}$$

From equation (31) we have,

$$\begin{aligned} a_m &= \chi_m a_{m-1} + hJ^{\alpha_1}[D_t^{\alpha_1} a_{m-1} + a_{m-1} - (\beta - \alpha) y_{m-1} \\ &\quad - \textstyle\sum_{i=0}^{m-1} a_i y_{m-1-i}] \\ y_m &= \chi_m y_{m-1} + hJ^{\alpha_2}[D_t^{\alpha_2} y_{m-1} - \tfrac{1}{\varepsilon} a_{m-1} + \tfrac{\beta}{\varepsilon} y_{m-1} \\ &\quad + \tfrac{1}{\varepsilon} \textstyle\sum_{i=0}^{m-1} a_i y_{m-1-i}] \end{aligned} \tag{25}$$

Consequently, the first few terms of the HAM

$$a_0 = 1, y_0 = 0,$$

$$a_1 = h \frac{t^{\alpha_1}}{\Gamma(\alpha_1+1)}, y_1 = -\frac{h}{\varepsilon} \frac{t^{\alpha_2}}{\Gamma(\alpha_2+1)},$$

$$a_2 = (h^2+h) \frac{t^{\alpha_1}}{\Gamma(\alpha_1+1)} + h^2 \frac{t^{2\alpha_1}}{\Gamma(2\alpha_1+1)} + \frac{h^2}{\varepsilon} (\beta - \alpha + 1) \frac{t^{\alpha_1+\alpha_2}}{\Gamma(\alpha_1+\alpha_2+1)},$$

$$y_2 = -\frac{1}{\varepsilon}(h^2+h) \frac{t^{\alpha_2}}{\Gamma(\alpha_2+1)} - \frac{h^2}{\varepsilon^2} (\beta+1) \frac{t^{2\alpha_2}}{\Gamma(2\alpha_2+1)} - \frac{h^2}{\varepsilon} \frac{t^{\alpha_1+\alpha_2}}{\Gamma(\alpha_1+\alpha_2+1)},$$

$$\begin{aligned} a_3 &= (h^3+2h^2+h) \tfrac{t^{\alpha_1}}{\Gamma(\alpha_1+1)} + (2h^3+2h^2) \tfrac{t^{2\alpha_1}}{\Gamma(2\alpha_1+1)} + h^3 \tfrac{t^{3\alpha_1}}{\Gamma(3\alpha_1+1)} + \\ &\tfrac{(\beta-\alpha+1)}{\varepsilon} (2h^3+2h^2) \tfrac{t^{\alpha_1+\alpha_2}}{\Gamma(\alpha_1+\alpha_2+1)} + \tfrac{h^3}{\varepsilon^2} (\beta - \alpha + 1)(\beta+1) \tfrac{t^{\alpha_1+2\alpha_2}}{\Gamma(\alpha_1+2\alpha_2+1)} \\ &+ \tfrac{h^3}{\varepsilon} \{2(\beta - \alpha + 1) + \tfrac{\Gamma(\alpha_1+\alpha_2+1)}{\Gamma(\alpha_1+1)\Gamma(\alpha_2+1)}\} \tfrac{t^{2\alpha_1+\alpha_2}}{\Gamma(2\alpha_1+\alpha_2+1)} \end{aligned}$$

$$\begin{aligned} y_3 &= -\tfrac{1}{\varepsilon}(h^3+2h^2+h) \tfrac{t^{\alpha_2}}{\Gamma(\alpha_2+1)} - \tfrac{(\beta+1)}{\varepsilon^2} (2h^3+2h^2) \tfrac{t^{2\alpha_2}}{\Gamma(2\alpha_2+1)} - \\ &\tfrac{h^3}{\varepsilon^3}(\beta+1)^2 \tfrac{t^{3\alpha_2}}{\Gamma(3\alpha_1+1)} - \tfrac{1}{\varepsilon}(2h^3+2h^2) \tfrac{t^{\alpha_1+\alpha_2}}{\Gamma(\alpha_1+\alpha_2+1)} - \tfrac{h^3}{\varepsilon} \tfrac{t^{2\alpha_1+\alpha_2}}{\Gamma(\alpha_1+2\alpha_2+1)} \\ &- \tfrac{h^3}{\varepsilon^2}\{2(\beta - \alpha + 1) + \tfrac{\Gamma(\alpha_1+\alpha_2+1)}{\Gamma(\alpha_1+1)\Gamma(\alpha_2+1)}\} \tfrac{t^{\alpha_1+2\alpha_2}}{\Gamma(\alpha_1+2\alpha_2+1)} \end{aligned}$$

Finally, we have

$$a(x,y,t) = \sum_{m=0}^{\infty} a_m(x,y,t), y(x,y,t) = \sum_{m=0}^{\infty} y_m(x,y,t) \tag{26}$$

Then

$$\begin{aligned} a_m &= 1 + (h^3+3h^2+3h) \tfrac{t^{\alpha_1}}{\Gamma(\alpha_1+1)} + (2h^3+3h^2) \tfrac{t^{2\alpha_1}}{\Gamma(2\alpha_1+1)} + h^3 \tfrac{t^{3\alpha_1}}{\Gamma(3\alpha_1+1)} + \\ &\tfrac{(\beta-\alpha+1)}{\varepsilon}(2h^3+3h^2) \tfrac{t^{\alpha_1+\alpha_2}}{\Gamma(\alpha_1+\alpha_2+1)} + \tfrac{h^3}{\varepsilon^2}(\beta - \alpha + 1)(\beta+1) \tfrac{t^{\alpha_1+2\alpha_2}}{\Gamma(\alpha_1+2\alpha_2+1)} \\ &+ \tfrac{h^3}{\varepsilon}\{2\beta - \alpha + 2 + \tfrac{\Gamma(\alpha_1+\alpha_2+1)}{\Gamma(\alpha_1+1)\Gamma(\alpha_2+1)}\} \tfrac{t^{2\alpha_1+\alpha_2}}{\Gamma(2\alpha_1+\alpha_2+1)} + \dots \end{aligned} \tag{27}$$

$$\begin{aligned} y_m &= -\tfrac{1}{\varepsilon}(h^3+3h^2+3h) \tfrac{t^{\alpha_2}}{\Gamma(\alpha_2+1)} - \tfrac{(\beta+1)}{\varepsilon^2}(2h^3+3h^2) \tfrac{t^{2\alpha_2}}{\Gamma(2\alpha_2+1)} - \\ &\tfrac{h^3}{\varepsilon^3}(\beta+1)^2 \tfrac{t^{3\alpha_2}}{\Gamma(3\alpha_1+1)} - \tfrac{1}{\varepsilon}(2h^3+3h^2) \tfrac{t^{\alpha_1+\alpha_2}}{\Gamma(\alpha_1+\alpha_2+1)} - \tfrac{h^3}{\varepsilon} \tfrac{t^{2\alpha_1+\alpha_2}}{\Gamma(2\alpha_1+\alpha_2+1)} \\ &- \tfrac{h^3}{\varepsilon^2}\{2\beta - \alpha + 2 + \tfrac{\Gamma(\alpha_1+\alpha_2+1)}{\Gamma(\alpha_1+1)\Gamma(\alpha_2+1)}\} \tfrac{t^{\alpha_1+2\alpha_2}}{\Gamma(\alpha_1+2\alpha_2+1)} - \dots. \end{aligned} \tag{28}$$

Equations (28) and (29) are solutions of fractional enzyme-catalyzed reaction model. For the purpose of comparing the analytical and numerical results, the following parameter values are used: $\alpha = 0.375$, $\beta = 1$ and $\varepsilon = 0.1$ which given from [**?**]. Respectively, Figure 1 shows that the convergence region of the series solution $-0.5 \le h \le -1.2$ and Figure 2 shows that in the initial stages, the concentration of the complex rises until it reaches a maximum. The results show that, our results when $\alpha_1 = \alpha_2 = 1$ are agreement with the result in [19]. See Table1 and Figure 1

5 Conclusions

We employ the HAM for finding the solutions of intermediate complex biochemical reaction model, and compare this solution with analytical and numerical solutions for different times. From the results we seen that HAM is a very powerful and efficient technique in finding analytical solutions for wide classes of systems of equations. They also do not require large computer memory, the results show that HAM is powerful mathematical tool for solving linear and nonlinear equations

Table 1: Comparison of the Homotopy Analysis Method, Direct Numerical Solutions and the Power Series for the Concentration of the Intermediate Complex, with$\alpha = 0.375$, $\beta = 1$, $\varepsilon = 0.1$ and *h*= -0.76.

t	Homotopy analysis solution y_{HAM}	Direct numerical solution y_N	Power series solution y_A
0.05	0.310507	0.310751	0.310727
0.075	0.37587	0.380089	0.379242
0.10	0.423122	0.421519	0.411202

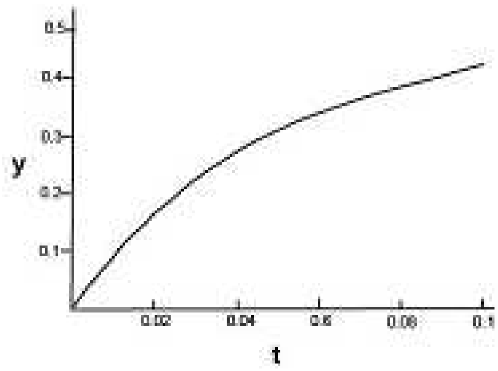

Fig. 1: *T*he h curve of $y'(0)$ obtained from HAM approximation solution of Eq.(29)

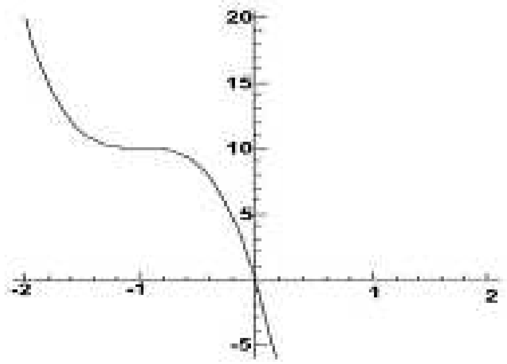

Fig. 2: The HAM solution for intermediate complex for Eq.(29) of *y(t)* in case of *h*=- 0.76, $\alpha_1 = \alpha_2 = 1$, and parameter values are used: $\alpha = 0.375, \beta = 1, \varepsilon = 0.1$

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