MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **90** (2023) 315–332
ISSN: 0340–6253
doi: 10.46793/match.90-2.315P

Kashuri Fundo Decomposition Method for Solving Michaelis-Menten Nonlinear Biochemical Reaction Model

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(Received January 5, 2023)

Abstract

In most of the real life problems, we encounter with nonlinear differential equations. Problems are made more understandable by modeling them with these equations. In this way, it becomes easier to interpret the problems and reach the results. In 1913, the basic enzymatic reaction model introduced by Michaelis and Menten to describe enzyme processes is an example of nonlinear differential equation. This model is the one of the simplest and best-known approaches of the mechanisms used to model enzyme-catalyzed reactions and is the most studied. For most nonlinear differential equations, it is very difficult to get an analytical solution. For this reason, various studies have been carried out to find approximate solutions to such equations. Among these studies, those in which two different methods are used by blending attract attention. In this study, a blended form of the Kashuri Fundo transform method and

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the Adomian decomposition method, so-called the Kashuri Fundo decomposition method, is used to find a solution to the Michaelis-Menten nonlinear biochemical reaction model in this way. This method has been applied to the biochemical reaction model and an approximate solution has been obtained for this model without complex calculations. This shows that the hybrid method is an effective, reliable, simpler and time-saving method in reaching the solutions of nonlinear differential equations.

1 Introduction

In most of the real life problems, we encounter with nonlinear differential equations. In 1913, the basic enzymatic reaction model introduced by Michaelis and Menten to describe enzyme processes is an example of nonlinear differential equations. This study made a great impression at the time of its publication and the proposed model has become a remarkable model in the biochemical field [13,37]. This article was first published in German and later translated into English [18, 38]. Biochemists often use the basic enyzmatic reaction model when analyzing enzyme kinetic parameters [5, 6, 20, 30, 47, 48].

The Michaelis Menten's nonlinear biochemical reaction model (BRM) scheme is modeled by in the form [46]

$$E + S \rightleftharpoons Y \rightarrow E + P \tag{1}$$

where E, S, Y and P represents the biomolecule that catalyzes (enzyme), the substance processed in the reaction (substrate), the intermediate complex and the product from the law of mass action, respectively. The basic enzymatic reaction model is the one of the simplest and best-known approaches of the mechanisms used to model enzyme-catalyzed reactions and is the most studied. In this model, a biomolecule that catalyzes and a substrate react to form an intermediate complex. This combination is reversible. This intermediate complex then decomposes into a product and regenerates the biomolecule that catalyzes. The transient phase of a reaction has an important place in determining various system parameters, and distinguishing between different mechanisms of enzyme catalysis, from a biochemical point of view [49].

By using the law of mass effect, the variation of equation (1) with time can be obtained by solving the following nonlinear coupled differential equations system [49].

$$\frac{dS}{dt} = -k_1 ES + k_{-1} Y \tag{2}$$

$$\frac{dE}{dt} = -k_1 ES + (k_{-1} + k_2) Y \tag{3}$$

$$\frac{dY}{dt} = k_1 ES - (k_{-1} + k_2) Y \tag{4}$$

$$\frac{dP}{dt} = k_2 Y \tag{5}$$

with the initial conditions

$$S(0) = S_0, \quad E(0) = E_0, \quad Y(0) = 0, \quad P(0) = 0 \tag{6}$$

where the parameters k_1 and k_{-1} are the positive rate constants of the forward and reverse reactions, respectively, expressed in model (1). k_2 is the positive rate constants of the forward reaction expressed in second step of model (1). Equations (2)-(5) can be rearranged and made more simple, for S and Y. These equations in the dimensionless form are given by [49]

$$\frac{ds}{dt} = -s + (\beta - \alpha) y + sy \tag{7}$$

$$\frac{dy}{dt} = \frac{1}{\epsilon}(s - \beta y - sy) \tag{8}$$

with the initial conditions

$$s(0) = 1, \quad y(0) = 0 \tag{9}$$

where s is the concentrations substrate and y is the intermediate complex between enzyme and substrate. α, β and ϵ are dimensionless parameters. For more detailed information on deriving equations (7) and (8), see reference [49].

Extracting analytic or approximate solutions for differential equations by using new analytic, semi-analytic or hybrid mathematical methods always attract the attention of the researchers due to the academic curiosity and practical applications. Adomian decomposition method (ADM) [1, 3, 25, 39, 56–59], homotopy perturbation method (HPM) [10, 21, 23, 24, 26–29, 36, 54, 55], variational iteration method (VIM) [4, 9, 22], Parker-Sochacki method (PSM) [2, 40, 45], modified Picard-Pade method (PPM) [35] and many different methods by which these methods are modified have been used in the solution of nonlinear differential equations such as BRM [7,8,19]. There exist several studies to compute the substrate concentration by numerically integrating the differential form of the Michaelis-Menten equation [16, 17, 60], by using root-solving techniques such as the bisection and Newton-Raphson methods in the integrated Michaelis-Menten equation [15]. Since a closed-form solution to the Michaelis-Menten equation is not available, motivation for having an accurate closed-form solution to this equation induces the possibility of analyzing the utility of other non-conventional solution techniques or methods to solve the Michaelis-Menten equation. In this study, we used a hybrid form of the Kashuri Fundo transform method [33] and the ADM, so-called the Kashuri Fundo decomposition method [52, 53], to find an approximate solution to the Michaelis-Menten nonlinear BRM.

Our main aim in this study is to demonstrate that Kashuri Fundo decomposition method is an effective, reliable, simpler and time-saving method that can be used in the solution of nonlinear differential equation systems. In order to demonstrate this, we use the basic enzymatic reaction model of Michaelis-Menten, which is modeled with nonlinear differential equation systems. First and foremost, we briefly mention the Kashuri Fundo transform and give its basic properties that are important for this study. Afterwards, we explain the procedure of application of the Kashuri Fundo decomposition method to a general form of a nonlinear differential equation. Consequently, this method is dealt with the basic enzymatic reaction model. Finally, we demonstrate the effectiveness of this method based on the process steps we have done. In the literature, it is possible to come across many studies in which Kashuri Fundo transform and its versions combined with different methods are used [11, 12, 14, 31, 32, 34, 41–

44, 50, 51].

2 Preliminaries

2.1 Kashuri Fundo Transform

2.1.1 Definition of Kashuri Fundo Transform

Definition 1. We consider functions in the set F defined [33],

$$F = \left\{ f(x) | \exists M, k_1, k_2 > 0 \quad \text{s.t.} \quad |f(x)| \leqslant M e^{\frac{|x|}{k_i^2}}, \quad \text{if} \quad x \in (-1)^i \times [0, \infty) \right\}$$

For a function belonging to the set F, M must be finite. k_1, k_2 may be finite or infinite.

Definition 2. Kashuri Fundo transform defined on the set F and denoted by $\mathscr{K}(.)$ is defined as [33],

$$\mathscr{K}[f(x)](v) = A(v) = \frac{1}{v} \int_0^\infty e^{\frac{-x}{v^2}} f(x)\, dx, \quad x \geqslant 0, \quad -k_1 < v < k_2. \quad (10)$$

The Kashuri Fundo transform expressed by equation (10) can also be expressed as [33],

$$\mathscr{K}[f(x)](v) = A(v) = v \int_0^\infty e^{-x} f(v^2 x)\, dx.$$

Definition 3. A function $f(x)$ is said to be of exponential order $\frac{1}{k^2}$, if there exist positive constants T and M such that $|f(x)| \leq M e^{\frac{-x}{k^2}}$, for all $x \geq T$ [33].

Theorem 1 (Sufficient Conditions for Existence of Kashuri Fundo Transform)**.** *If $f(x)$ is piecewise continuous on $[0, \infty)$ and of exponential order $\frac{1}{k^2}$, then $\mathscr{K}[f(x)](v)$ exists for $|v| < k$ [33].*

2.1.2 Some Properties of Kashuri Fundo Transform

Theorem 2 (Linearity of Kashuri Fundo Transform)**.** *Let $f(x)$ and $g(x)$ be functions whose Kashuri Fundo integral transforms exist and c be a constant. Then [33],*

1. $\mathscr{K}[(f+g)(x)](v) = \mathscr{K}[f(x)](v) + \mathscr{K}[g(x)](v)$

2. $\mathscr{K}[(cf)(x)](v) = c\mathscr{K}[f(x)](v)$

Theorem 3 (Kashuri Fundo Transform of The Derivatives)**.** *Let's assume that the Kashuri Fundo transform of $f(x)$, denoted by $A(v)$, exists. Then [33],*

$$\mathscr{K}\left[\frac{df(x)}{dx}\right](v) = \frac{A(v)}{v^2} - \frac{f(0)}{v} \tag{11}$$

$$\mathscr{K}\left[\frac{d^2f(x)}{dx^2}\right](v) = \frac{A(v)}{v^4} - \frac{f(0)}{v^3} - \frac{f'(0)}{v} \tag{12}$$

$$\mathscr{K}\left[\frac{d^{(n)}f(x)}{dx^{(n)}}\right](v) = \frac{A(v)}{v^{2n}} - \sum_{k=0}^{n-1} \frac{f^{(k)}(0)}{v^{2(n-k)-1}} \tag{13}$$

2.2 Kashuri Fundo Decomposition Method

Consider a nonlinear differential equation written in a general operator form

$$Lz(t) + Rz(t) + Nz(t) = g(t) \tag{14}$$

with initial condition

$$z(0) = c, \quad (c \in \mathbb{R})$$

where L is the highest-order derivative which is assumed to be invertible, R is a linear differential operator of less order than L, N is the nonlinear operator and g is the source term. z is a function dependent on the variable t.

Kashuri Fundo decomposition method is as follows [52, 53]:

By applying the Kashuri Fundo transform to the expression in equation

Table 1. Kashuri Fundo transform of some special functions [33, 52]

$f(x)$	$A(v)$
1	v
x	v^3
$x^n, \quad n \in \mathbb{Z}$	$n! v^{2n+1}$
e^{cx}	$\frac{v}{1-cv^2}$
$sin(cx)$	$\frac{cv^3}{1+c^2v^4}$
$cos(cx)$	$\frac{v}{1+c^2v^4}$
$sinh(cx)$	$\frac{cv^3}{1-c^2v^4}$
$cosh(cx)$	$\frac{v}{1-c^2v^4}$
$x^\alpha, \quad \alpha \in \mathbb{R}^+$	$\Gamma(\alpha+1) v^{2\alpha+1}$
$\sum\limits_{k=0}^{n} c_k x^k$	$\sum\limits_{k=0}^{n} k! c_k v^{2k+1}$

(14) and using equation (11), we get

$$z(v) = cv + v^2 \mathscr{K}[g(t)] - v^2 \mathscr{K}[Rz(t)] - v^2 \mathscr{K}[Nz(t)] \tag{15}$$

Having applied bilaterally the inverse of Kashuri Fundo transform to this new equation, we acquire

$$z(t) = c + \mathscr{K}^{-1}\left[v^2 \mathscr{K}[g(t)]\right] - \mathscr{K}^{-1}\left[v^2 \mathscr{K}[Rz(t)]\right] - \mathscr{K}^{-1}\left[v^2 \mathscr{K}[Nz(t)]\right] \tag{16}$$

When equation (16) is carefully examined, it can be seen that it is very difficult to obtain the inverse Kashuri Fundo transforms of some expressions in the equation. This difficulty can be overcome by using the ADM from this stage of the solution. The ADM is based on the assumption that the $z(t)$ function can be expressed as an infinite series.

$$z(t) = \sum_{n=0}^{\infty} z_n(t) = z_0 + z_1 + z_2 + z_3 + \dots \tag{17}$$

where z_n can be determined iteratively. In the ADM, nonlinear Nz can also be expressed as an infinite polynomial series.

$$Nz = \sum_{n=0}^{\infty} A_n \tag{18}$$

The expression A_n in equation (18) consists of $A_n(z_0, z_1, z_2, z_3, \ldots, z_n)$ and is called the Adomian polynomials.

$$A_n(z_0, z_1, z_2, z_3, \ldots, z_n) = \frac{1}{n!}\frac{d^n}{d\lambda^n}\left[N\left(\sum_{k=0}^{n} \lambda^k z_k\right)\right]_{\lambda=0}, \quad n = 0, 1, 2, \ldots$$

where λ is a parameter. The Adomian polynomials A_n is defined as

$$\begin{aligned}
A_0 &= \frac{1}{0!}\frac{d^0}{d\lambda^0}\left[N\left(\sum_{k=0}^{0} \lambda^k z_k\right)\right]_{\lambda=0} = N(z_0)\\
A_1 &= \frac{1}{1!}\frac{d^1}{d\lambda^1}\left[N\left(\sum_{k=0}^{1} \lambda^k z_k\right)\right]_{\lambda=0} = z_1 N'(z_0)\\
A_2 &= \frac{1}{2!}\frac{d^2}{d\lambda^2}\left[N\left(\sum_{k=0}^{2} \lambda^k z_k\right)\right]_{\lambda=0} = z_2 N'(z_0) + \frac{z_1^2}{2!}N''(z_0)\\
&\vdots
\end{aligned}$$

Substituting the equations (17) and (18) into the equation (16), we find

$$\begin{aligned}
\sum_{n=0}^{\infty} z_n(t) = c + \mathscr{K}^{-1}\left[v^2 \mathscr{K}[g(t)]\right] - \mathscr{K}^{-1}\left[v^2 \mathscr{K}\left[R \sum_{n=0}^{\infty} z_n(t)\right]\right]\\
- \mathscr{K}^{-1}\left[v^2 \mathscr{K}\left[\sum_{n=0}^{\infty} A_n\right]\right]
\end{aligned} \tag{19}$$

Describing both sides of (19) will successively produce

$$
\begin{aligned}
z_0 &= c + \mathscr{K}^{-1}\big[v^2\mathscr{K}[g(t)]\big] \\
z_1 &= -\mathscr{K}^{-1}\big[v^2\mathscr{K}[Rz_0]\big] - \mathscr{K}^{-1}\big[v^2\mathscr{K}[A_0]\big] \\
z_2 &= -\mathscr{K}^{-1}\big[v^2\mathscr{K}[Rz_1]\big] - \mathscr{K}^{-1}\big[v^2\mathscr{K}[A_1]\big] \\
z_3 &= -\mathscr{K}^{-1}\big[v^2\mathscr{K}[Rz_2]\big] - \mathscr{K}^{-1}\big[v^2\mathscr{K}[A_2]\big] \\
&\vdots
\end{aligned}
$$

Thus, the solution of equation (14) is obtained recursively by the Kashuri Fundo decomposition method as follows

$$
\begin{aligned}
z_0 &= c + \mathscr{K}^{-1}\big[v^2\mathscr{K}[g(t)]\big] \\
z_{n+1} &= -\mathscr{K}^{-1}\big[v^2\mathscr{K}[Rz_n]\big] - \mathscr{K}^{-1}\big[v^2\mathscr{K}[A_n]\big].
\end{aligned}
$$

As a result, the general expression of the approximate solution is expressed as

$$
z \approx \sum_{n=0}^{k} z_n, \quad \text{where} \quad \lim_{k\to\infty} \sum_{n=0}^{k} z_n = z.
$$

3 Main Result

3.1 Application to The Biochemical Reaction Model

Applying the Kashuri Fundo transform to equations (7) and (8), we find

$$
\mathscr{K}\left[\frac{ds}{dt}\right] = \mathscr{K}[-s + (\beta - \alpha)y + sy] \tag{20}
$$

$$
\mathscr{K}\left[\frac{dy}{dt}\right] = \frac{1}{\epsilon}\mathscr{K}[s - \beta y - sy] \tag{21}
$$

where

$$
\begin{aligned}
\mathscr{K}\left[\frac{ds}{dt}\right] &= \frac{\mathscr{K}[s(t)]}{v^2} - \frac{s(0)}{v} \\
&= \frac{\mathscr{K}[s(t)]}{v^2} - \frac{1}{v}
\end{aligned} \tag{22}
$$

$$\begin{aligned}\mathscr{K}\left[\frac{dy}{dt}\right] &= \frac{\mathscr{K}[y(t)]}{v^2} - \frac{y(0)}{v} \\ &= \frac{\mathscr{K}[y(t)]}{v^2}\end{aligned} \tag{23}$$

Substituting these equations into the equations (20) and (21), we get

$$\frac{\mathscr{K}[s(t)]}{v^2} - \frac{1}{v} = \mathscr{K}[-s + (\beta - \alpha)y + sy] \tag{24}$$

$$\frac{\mathscr{K}[y(t)]}{v^2} = \frac{1}{\epsilon}\mathscr{K}[s - \beta y - sy] \tag{25}$$

$$\mathscr{K}[s(t)] = v + v^2\mathscr{K}[-s + (\beta - \alpha)y + sy] \tag{26}$$

$$\mathscr{K}[y(t)] = v^2\frac{1}{\epsilon}\mathscr{K}[s - \beta y - sy] \tag{27}$$

Applying the inverse Kashuri Fundo transform in equations (26) and (27), we get

$$s(t) = 1 + \mathscr{K}^{-1}\left[v^2\mathscr{K}[-s + (\beta - \alpha)y + sy]\right] \tag{28}$$

$$y(t) = \mathscr{K}^{-1}\left[v^2\frac{1}{\epsilon}\mathscr{K}[s - \beta y - sy]\right] \tag{29}$$

Assuming the solution is an infinite series of unknown functions, we can write

$$s(t) = \sum_{m=0}^{\infty} s_m(t) \quad \text{ve} \quad y(t) = \sum_{m=0}^{\infty} y_m(t)\ , \quad \sum_{m=0}^{\infty} A_m = sy$$

Arranging equations (28) and (29) according to this assumption, we get

$$\sum_{m=0}^{\infty} s_m(t) = 1 + \mathscr{K}^{-1}\left[v^2\mathscr{K}\left[-\sum_{m=0}^{\infty} s_m(t) + (\beta - \alpha)\sum_{m=0}^{\infty} y_m(t) + \sum_{m=0}^{\infty} A_m\right]\right] \tag{30}$$

$$\sum_{m=0}^{\infty} y_m(t) = \mathscr{K}^{-1}\left[v^2\frac{1}{\epsilon}\mathscr{K}\left[\sum_{m=0}^{\infty} s_m(t) - \beta\sum_{m=0}^{\infty} y_m(t) - \sum_{m=0}^{\infty} A_m\right]\right] \tag{31}$$

where A_m is Adomian polynomials and is given as follows

$$A_0 = s_0 y_0 \ , \ A_1 = s_0 y_1 + s_1 y_0 \ , \ A_2 = s_0 y_2 + s_1 y_1 + s_2 y_0 \ , \ \ldots$$

We can write the equations (30) and (31) for the values of m as

$$s_0(t) = 1 \tag{32}$$

$$s_1(t) = \mathscr{K}^{-1}\left[v^2 \mathscr{K}\left[-s_0(t) + (\beta - \alpha) y_0(t) + A_0\right]\right] \tag{33}$$

$$\vdots$$

$$s_{k+1}(t) = \mathscr{K}^{-1}\left[v^2 \mathscr{K}\left[-s_k(t) + (\beta - \alpha) y_k(t) + A_k\right]\right] \tag{34}$$

$$y_0(t) = 0 \tag{35}$$

$$y_1(t) = \mathscr{K}^{-1}\left[v^2 \frac{1}{\epsilon} \mathscr{K}\left[s_0(t) - \beta y_0(t) - A_0\right]\right] \tag{36}$$

$$\vdots$$

$$y_{k+1}(t) = \mathscr{K}^{-1}\left[v^2 \frac{1}{\epsilon} \mathscr{K}\left[s_k(t) - \beta y_k(t) - A_k\right]\right] \tag{37}$$

Thus, the solution of equations (7) and (8) is obtained recursively using the Kashuri Fundo decomposition method. We can express this approximate solution in general as follows

$$S_m(t) = \sum_{m=0}^{\infty} s_m(t) = s_0(t) + s_1(t) + s_2(t) + \ldots \tag{38}$$

$$Y_m(t) = \sum_{m=0}^{\infty} y_m(t) = y_0(t) + y_1(t) + y_2(t) + \ldots \tag{39}$$

If we assume that $\alpha = 0.375$, $\beta = 1$ and $\epsilon = 0.1$, we get

$$s(t) = 1 - t + 8.625t^2 - 63.0833t^3 + \ldots \tag{40}$$

$$y(t) = 10t - 105t^2 + 762.083t^3 - \ldots \tag{41}$$

This result coincides with the results found in references [2, 4, 8, 35]. The graphs of the equations (40) and (41) up to the third order are shown in figures 1 and 2, respectively. Figure 3 shows the behavior of these equations together.

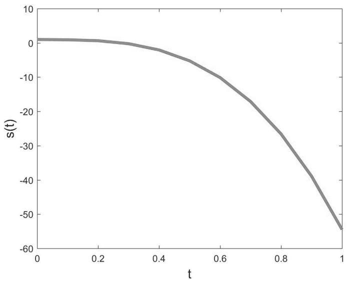

Figure 1. The graph of $s(t)$.

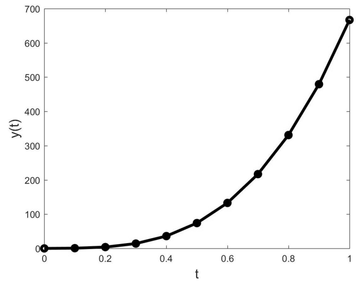

Figure 2. The graph of $y(t)$.

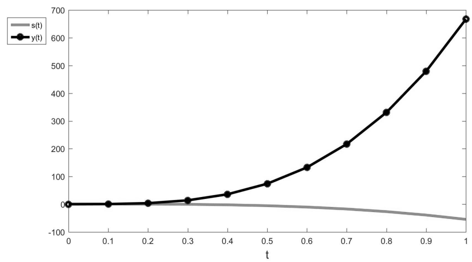

Figure 3. The behavior of $s(t)$ and $y(t)$.

4 Conclusion

Differential equations allow us to understand the phenomena in the background by modeling the events we experience in our life. This feature makes it important to reach the solutions of this type of equations. Especially, reaching the solutions of nonlinear differential equations can be quite complex and time consuming in some cases. In order to prevent this confusion and waste of time, many different methods have been put forward. In this study, we examined the effectiveness of Kashuri Fundo decomposition method, based on Michaelis-Menten's basic enzymatic reaction model. In the application of the Kashuri Fundo decomposition method to this model, we first transform the system of equations into algebraic form by using the Kashuri Fundo transform. Then, by implementing the Adomian decomposition method for nonlinear term, we obtained the solution starting from the assumption that the solution is an infinite series of unknown functions. When we examined the process steps that we made using the Kashuri Fundo decomposition method, we revealed to the conclusion that we obtained a solution in a short time and with fewer process steps compared to studies in the literature, without going through complex calculations, without the need for any computer program. As a result, we present an approach that provides a series solution of any desired accuracy through an appropriate selection of solution order for the Michaelis-Menten equation. The solution found by the proposed hybrid method is algebraic in nature and is valid for all values of substrate concentration and kinetic parameters. It does not rely on a (large or small) parameter. Therefore, one of the significant features of this solution is the fact that it takes the place of numerical solutions with the evaluation of simple algebraic expressions. Hence, the algebraic nature of the obtained series solution and its high accuracy make this proposed hybrid method an attractive candidate for computing substrate concentration and intermediate complex in the Michaelis-Menten equation. In the light of these facts, it is possible to say that the Kashuri Fundo decomposition method is an effective, reliable, useful and time-saving method that can be used in the solution of nonlinear differential equation systems.

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