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Research article

Computational analysis of fractional Michaelis-Menten enzymatic reaction model

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Abstract: In this study for examining the fractional Michaelis-Menten enzymatic reaction (FMMER) model, we suggested a computational method by using an operational matrix of Jacobi polynomials (JPs) as its foundation. We obtain an operational matrix for the arbitrary order derivative in the Caputo sense. The fractional differential equations (FDEs) are then reduced to a set of algebraic equations by using attained operational matrix and the collocation method. The approach which utilized in this study is quicker and more effective compared to other schemes. We also compared the suggested method with the Vieta-Lukas collocation technique (VLCM) and we obtain excellent results. A comparison between numerical outcomes is shown by figures and tables. Error analysis of the recommended methods is also presented.

Keywords: FMMER; VLCM; Jacobi polynomials; FDEs; operational matrix; collocation technique
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1. Introduction

Fractional-order differential equations allow scientists to simulate a wide range of physical phenomena. To solve systems by creating precise models, arbitrary-order differential operators are frequently utilized [1–4]. Due of their property that is not local, the arbitrary-order operators are more effective at simulating the different issues in physics, fluid dynamics, and the associated fields [1,5–9].

To investigate the approximation of the Michaelis-Menten enzymatic reaction equation, Shateyi et al. [10] recommended a technique that is modification of the spectral homotopy analysis technique. To get the best design of several membrane reactors operating enzyme-catalyzed reactions in series, Abu-Reesh [11] deduced analytical equations. A precise closed-form resolution to the Michaelis-Menten equation using the terms of Lambert W(x) function was proposed by Golicnik [12]. Hussam et al. [13] utilized the Laplace transformation and Adomian decomposition method to examine the semianalytical outcomes of fractional time enzyme kinetics. Alqhtani et al. [14] suggested a scale conjugate neural network learning procedure for the non linear malaria illness concept. Numerous researchers have shown computational, estimate techniques and applications to address this issue because it can be challenging to find exact solutions to arbitrary order differential equations [15–19]. In actuality, aside from [20], no other techniques cope with computational solutions in the fractal-fractional sense. The authors of [21] examined a spectral approach in the context of fractal-fractional differentiation.

Alqhtani and Saad [22] examined the fractal-fractional michaelis-menten enzymatic reaction model using different kernels. Alsuyuti et al. [23] investigated the Galerkin operational technique for multi-dimension fractional differential equations. Spectral Galerkin schemes for a class of multi-order fractional pantograph equations was examined by Alsuyuti et al. [24]. Bhrawy et al. [25] studied an effective spectral collocation technique for a dual-sided spaces fractional Boussinesq equation having non-local circumstances. According to Michaelis and Menten, the enzyme-substrate complex quantity estimated by the Michaelis-Menten equations [26] is proportional to the rate of an enzyme-catalyzed process. [26] illustrates this model's dynamic version:

$$\frac{d\varepsilon}{dt} = -\omega\varepsilon(t)\varphi(t) + \chi\varrho(t), \tag{1}$$

$$\frac{d\varphi}{dt} = -\omega\varepsilon(t)\varphi(t) + (\chi + \beta)\varrho(t), \tag{2}$$

$$\frac{d\varrho}{dt} = \omega\varepsilon(t)\varphi(t) - (\chi + \beta)\varrho(t), \tag{3}$$

$$\frac{d\vartheta}{dt} = \beta\varrho(t). \tag{4}$$

The substrate's concentration is represented by $\varepsilon(t)$, and an enzyme's concentration is $\varphi(t)$. The resulting complex's concentration is $\varrho(t)$, and the resulting product's concentration is represented by $\vartheta(t)$. ω, χ and β represent the reaction rate regarding the complex's production from $\varepsilon(t)$ and $\varphi(t)$, the rate of reaction governing the complex's breakdown to $\varphi(t)$ and $\varphi(t)$, and the reaction rate governing the complex's breaking down into $\vartheta(t)$ and $\varphi(t)$ respectively. Initial conditions are $\varepsilon(0) = \varepsilon_0$, $\varphi(0) = \varphi_0$, $\varrho(0) = \varrho_0$ and $\vartheta(0) = \vartheta_0$.

The schematic for this model is provided by

$$\varepsilon + \varphi \rightleftharpoons \varrho \rightarrow \varphi + \vartheta.$$

This diagram shows that an enzyme φ and a substrate ε react to produce a complex ϱ. In the end, an enzyme ϑ and a product φ are produced from a complex ϱ [22].

In this article, we presented the computational solution of the FMMER model by Jacobi collocation method (JCM) and VLCM. It should be mentioned that the FMMER model is handled originally in

this study using the collocation strategy. It is important to note that no have comparable works that apply this technique to issues regarding the FMMER model.

2. Preliminaries

2.1. Overview of fractional calculus

Here, we provide a summary of some definitions, characteristics, and outcomes related to fractional calculus, which is important for developing the computational technique used to resolve FDEs.

Definition 1. The definition of the Riemann-Liouville fractional integral operator of a function ψ of order $\nu > 0$ is

$$J^{\nu}\psi(z) = \frac{1}{\Gamma(\nu)}\int_0^z (z-s)^{\nu-1}\psi(s)ds, \quad \nu > 0,$$
$$J^{0}\psi(z) = \psi(z).$$

Definition 2. The definition of fractional derivative in Caputo sense for order ν is

$$D^{\nu}\psi(z) = \frac{1}{\Gamma(n-\nu)}\int_0^z \frac{\psi^{(n)}(s)}{(z-s)^{\nu+1-n}}ds, \quad \nu > 0,\ z > 0,$$

where $n-1 < \nu \leq n$, $n \in \mathbb{N}$ and $\psi \in C^n[0,1]$. So, the Caputo operator follows

$$D^{\nu}z^k = \begin{cases} 0, & k \in 0, 1, 2, \cdots, \lceil \nu \rceil - 1, \\ \frac{\Gamma(1+k)}{\Gamma(1+k-\nu)}z^{k-\nu}, & k \in \mathbb{N} \wedge k \geq \lceil \nu \rceil. \end{cases}$$

To learn more about the definitions of fractional derivatives and their characteristics, see [27, 28]. The derivatives d/dt are replaced in the dimensionless enzymatic reaction Eqs (1)–(4) by the fractional derivatives D^{ν}, $0 < \nu \leq 1$. Thus, we attain the fractional model is

$$D^{\nu}\varepsilon(t) = -\omega\varepsilon(t)\varphi(t) + \chi\varrho(t), \tag{5}$$
$$D^{\nu}\varphi(t) = -\omega\varepsilon(t)\varphi(t) + (\chi+\beta)\varrho(t), \tag{6}$$
$$D^{\nu}\varrho(t) = \omega\varepsilon(t)\varphi(t) - (\chi+\beta)\varrho(t), \tag{7}$$
$$D^{\nu}\vartheta(t) = \beta\varrho(t). \tag{8}$$

2.2. JPs

In this article, JPs have served as the foundation for approximating unknown functions. The shifted JPs is defined as [29–31]

$$j_r^{(p,q)}(z) = \sum_{w=0}^{r}(-1)^{r-w}\frac{\Gamma(r+q+1)\Gamma(r+w+p+q+1)}{\Gamma(w+q+1)\Gamma(r+p+q+1)(r-w)!w!}z^w,$$

the JPs parameters, p and q, are as stated in [29].

The following are orthogonal properties of JPs:

$$\int_0^1 j_k^{(p,q)}(z)j_s^{(p,q)}(z)\omega^{(p,q)}(z)dz = \lambda_k^{p,q}\delta_{ks},$$

δ_{ks} is Kronecker delta function and $\omega^{(p,q)}(z)$ is a weight function and presented as

$$\omega^{(p,q)}(z) = (1-z)^p z^q$$

and

$$\lambda_k^{p,q} = \frac{\Gamma(k+p+1)\Gamma(k+q+1)}{(2k+p+q+1)k!\Gamma(k+p+q+1)}.$$

2.3. Operational matrix of JPs for fractional derivative

Theorem 1. Suppose that the shifted Jacobi vector is

$$J_k(z) = [j_0^{(p,q)}, j_1^{(p,q)}, \cdots, j_k^{(p,q)}]^T$$

and $\nu > 0$. Then

$$D^\nu j_r^{(p,q)}(z) = D^{(\nu)} J_k(z),$$

here $D^{(\nu)} = (N(r,i))$ is operational matrix of $(k+1)\times(k+1)$ order and ν denotes order of fractional derivative , whose entries are offered as

$$\begin{aligned} N(r,i,p,q) &= \sum_{l=[\nu]}^{r}(-1)^{r-l}\frac{\Gamma(r+q+1)\Gamma(r+l+p+q+1)}{(r-l)!\Gamma(l+q+1)\Gamma(r+p+q+1)\Gamma(l-\nu+1)} \\ &\times \sum_{e=0}^{i}(-1)^{i-e}\frac{\Gamma(p+1)\Gamma(i+e+p+q+1)\Gamma(l+e-\nu+q+1)(2i+p+q+1)i!}{(i-e)!(e)!\Gamma(i+p+1)\Gamma(e+q+1)\Gamma(l+e-\nu+p+q+2)}. \end{aligned}$$

Proof. [29–31] are available to view as evidence. □

2.4. Function approximation for JCM

A function $\eta \in L_f^2[0,1]$, with $|\eta"(z)| \le A$, can be expanded as

$$\eta(z) = \lim_{k\to\infty}\sum_{r=0}^{k} a_r j_r^{(p,q)}(z), \quad \eta(z) =< a_r, j_r^{(p,q)}(z) >, \tag{9}$$

where the standard inner product space is indicated by the sign $< ., . >$.

For the estimation of finite dimensions, the composition of Eq (9) is as follows:

$$\eta \cong \sum_{r=0}^{m} a_r j_r^{(p,q)}(z) = A^T J_m(z), \tag{10}$$

where A and $J_m(z)$ are matrices of order $(m+1)\times 1$, presented as

$$A = [a_0, a_1, ..., a_m]^T \quad \text{and} \quad J_m(z) = [j_0^{(p,q)}, j_1^{(p,q)}, \cdots, j_m^{(p,q)}]^T. \tag{11}$$

2.5. Vieta-Lukas polynomials (VLPs)

Shifted VLPs on [0,1], in analytical form, can be written as [32]

$$v_r(z) = 2r\sum_{j=0}^{r}(-1)^j\frac{4^{r-j}\Gamma(2r-j)}{\Gamma(j+1)\Gamma(2r-2j+1)}z^{r-j}, \quad r = \{2,3,\cdots\}$$

with $v_0(z) = 2$.

2.6. Operational matrix of VLPs for fractional derivative

Theorem 1. Suppose that the shifted Vieta-Lukas vector is

$$V_k(z) = [v_0, v_1, ..., v_k]^T$$

and $\nu > 0$. Then,

$$D^{\nu} v_r(z) = D^{(\nu)} V_k(z),$$

here $D^{(\nu)}$ is an operational matrix of order $(k+1) \times (k+1)$ and ν represents the order of the fractional derivative, the entries of which are provided in [32].

$$D^{(\nu)} = \begin{pmatrix} 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \cdots & \vdots \\ 0 & 0 & \cdots & 0 \\ \sum_{m=0}^{i-\lceil \nu \rceil} \sigma_{i,0,m} & \sum_{m=0}^{i-\lceil \nu \rceil} \sigma_{i,1,m} & \cdots & \sum_{m=0}^{i-\lceil \nu \rceil} \sigma_{i,k,m} \\ \vdots & \vdots & \cdots & \vdots \\ \sum_{m=0}^{k-\lceil \nu \rceil} \sigma_{k,0,m} & \sum_{m=0}^{k-\lceil \nu \rceil} \sigma_{k,1,m} & \cdots & \sum_{m=0}^{k-\lceil \nu \rceil} \sigma_{k,k,m} \end{pmatrix}$$

and $\sigma_{i,j,m}$ is given by

$$\sigma_{i,j,m} = \begin{cases} i \sum_{m=0}^{i-\lceil \nu \rceil} (-1)^m \frac{4^{i-m}\Gamma(2i-m)\Gamma(i-m+1)\Gamma(i-m-\nu+1/2)}{\sqrt{\pi}\Gamma(m+1)\Gamma(2i-2m+1)\Gamma(i-m-\nu+1)^2}, & j = 0, \\ 2i \sum_{m=0}^{i-\lceil \nu \rceil} \sum_{r=0}^{j} \frac{(-1)^{m+r}}{\sqrt{\pi}} \frac{4^{i-m}\Gamma(2i-m)\Gamma(i-m+1)}{\Gamma(m+1)\Gamma(2i-2m+1)\Gamma(i-m-\nu+1)} \times \frac{4^{j-r}\Gamma(2j-r)\Gamma(i+j-m-r-\nu+1/2)}{\Gamma(r+1)\Gamma(2j-2r+1)\Gamma(i+j+m-r-\nu+1)}, & j = 1, 2, 3, \cdots. \end{cases}$$

Proof. See [32]. □

2.7. Function approximation for VLCM

A function $\rho \in L^2_f[0,1]$, with $|\rho"(z)| \leq A$, can be expanded in this way:

$$\rho(z) = \lim_{k \to \infty} \sum_{r=0}^{k} b_r v_r(z), \tag{12}$$

where

$$b_r = \frac{1}{\mu_r \pi} \int_0^1 \frac{\rho(z) v_r(z)}{\sqrt{z - z^2}} dz,$$

$\mu_0 = 4$ and $\mu_r = 2$ $(r \geq 1)$.

Regarding estimate of finite dimensions, this is the composition of Eq (12):

$$\rho \cong \sum_{r=0}^{m} b_r v_r(z) = C^T V_m(z), \tag{13}$$

where shifted VLPs coefficient C and shifted VLP vector $V_m(z)$ [matrices of order $(m+1) \times 1$] are

$$C = [b_0, b_1, \cdots, b_m]^T \quad \text{and} \quad V_m(z) = [v_0, v_1, \cdots, v_m]^T. \tag{14}$$

3. Overview of the JCM method

Here, we will review the algorithm that uses the operational matrix and collocation strategy [33–35] to generate the solution for the FDEs. We utilize the subsequent approximation:

$$\pi(t) = \sum_{r=0}^{k} a_r j_r^{(p,q)}(t) = A^T J_k(t). \tag{15}$$

Next, by taking the derivative of (15) at order one, we arrive at

$$D'\pi(t) = A^T D' J_k(t) \cong A^T D^{(1)} J_k(t), \tag{16}$$

where $D^{(1)}$ is the operational differentiation matrix of order 1 for JPs.

Taking the order ν derivative of (15), we get

$$D^{\nu}\pi(t) = A^T D^{\nu} J_k(t) \cong A^T D^{(\nu)} J_r(t), \tag{17}$$

where $D^{(\nu)}$ is the operational differentiation matrix of order ν for JPs.

Eqations (15) and (16) allow us to write

$$\pi(0) = A^T J_k(0), \tag{18}$$

$$\pi'(0) = A^T D^{(1)} J_k(0). \tag{19}$$

4. Numerical simulation of the FMMER model by JCM

Grouping Eqs (5), (15) and (17), we obtain

$$A_1^T D^{(\nu)} J_k(t) + \omega(A_1^T J_k(t))(A_2^T J_k(t)) - \chi(A_3^T J_k(t)) = 0. \tag{20}$$

Grouping Eqs (6), (15) and (17), we obtain

$$A_2^T D^{(\nu)} J_k(t) + \omega(A_1^T J_k(t))(A_2^T J_k(t)) - (\chi + \beta)(A_3^T J_k(t)) = 0. \tag{21}$$

Grouping Eqs (7), (15) and (17), we obtain

$$A_3^T D^{(\nu)} J_k(t) - \omega(A_1^T J_k(t))(A_2^T J_k(t)) + (\chi + \beta)(A_3^T J_k(t)) = 0. \tag{22}$$

Grouping Eqs (8), (15) and (17), we obtain

$$A_4^T D^{(\nu)} J_k(t) - \beta(A_3^T J_k(t)) = 0. \tag{23}$$

The residual for Eqs (20)–(23) are given as follows:

$$R_{1k}(t) = A_1^T D^{(\nu)} J_k(t) + \omega(A_1^T J_k(t))(A_2^T J_k(t)) - \chi(A_3^T J_k(t)), \tag{24}$$

$$R_{2k}(t) = A_2^T D^{(\nu)} J_k(t) + \omega(A_1^T J_k(t))(A_2^T J_k(t)) - (\chi + \beta)(A_3^T J_k(t)), \tag{25}$$

$$R_{3k}(t) = A_3^T D^{(\nu)} J_k(t) - \omega(A_1^T J_k(t))(A_2^T J_k(t)) + (\chi + \beta)(A_3^T J_k(t)), \tag{26}$$

$$R_{4k}(t) = A_4^T D^{(\nu)} J_k(t) - \beta(A_3^T J_k(t)). \tag{27}$$

Now, when Eqs (24)–(27) are collocated at k points

$$t_r = \frac{r}{k}, \quad r = 0, 1, 2, \cdots, k-1,$$

we obtain

$$R_{1k}(t_r) = A_1^T D^{(\nu)} J_k(t_r) + \omega(A_1^T J_k(t_r))(A_2^T J_k(t_r)) - \chi(A_3^T J_k(t_r)), \tag{28}$$

$$R_{2k}(t_r) = A_2^T D^{(\nu)} J_k(t_r) + \omega(A_1^T J_k(t_r))(A_2^T J_k(t_r)) - (\chi + \beta)(A_3^T J_k(t_r)), \tag{29}$$

$$R_{3k}(t_r) = A_3^T D^{(\nu)} J_k(t_r) - \omega(A_1^T J_k(t_r))(A_2^T J_k(t_r)) + (\chi + \beta)(A_3^T J_k(t_r)), \tag{30}$$

$$R_{4k}(t_r) = A_4^T D^{(\nu)} J_k(t_r) - \beta(A_3^T J_k(t_r)). \tag{31}$$

Furthermore, from Eq (18), we can write

$$A_1^T J_k(0) - \varepsilon(0) = 0, \tag{32}$$

$$A_2^T J_k(0) - \varphi(0) = 0, \tag{33}$$

$$A_3^T J_k(0) - \varrho(0) = 0, \tag{34}$$

$$A_4^T J_k(0) - \vartheta(0) = 0. \tag{35}$$

By using the collocation points in Eqs (28)–(31), along with Eqs (32)–(35), we are left with a non-linear system of equations that have the same amount of unknowns. The estimated solution of the FMMER model is obtained by solving this system.

5. Analysis of the plan for JCM

Theorem 5.1. Define the function as π: $[0, 1] \longrightarrow R$, $\pi \in C^{(k+1)}[0, 1]$, where the k^{th} estimate found using JPs is $\pi_k(z)$. Then,

$$F_{\pi,k}^h = ||\pi - \pi_k||_{L_h^2[0,1]}, \tag{36}$$

and as $k \longrightarrow \infty$, the error vector $F_{\pi,k}^h \longrightarrow 0$.

Proof. For evidence, consult the relevant books [36, 37], and the study article [38]. □

Theorem 5.2. The error vector for ν order operational matrix differentiation is $F_{D,k}^{\nu,h}$, and it is computed utilizing $(k + 1)$ JPs. Then,

$$F_{D,k}^{\nu,h} = D^{(\nu)} J_k(t) - D^{\nu} J_k(t), \tag{37}$$

and as $k \longrightarrow \infty$, $F_{D,k}^{\nu,h} \longrightarrow 0$.

Proof. [39, 40] are available for viewing. □

Theorem 5.3. Consider the functional Y. Then

$$\lim_{k\to\infty} \zeta_k(t) = \zeta(t) = \inf_{t\in[0,1]} Y(t). \tag{38}$$

Proof. See [41]. For Eq (5), the functional Y is offered as

$$Y(t) = D_t^{\gamma}\varepsilon(t) + \omega\varepsilon(t)\varphi(t) + \chi\varrho(t). \tag{39}$$

Using Eqs (15) and (17), we obtain

$$Y^{(F)}(t) = A_1^T D^{(\nu)} Y_k(t) + F_{D,k}^{\nu,h} + \omega(A_1^T J_k(t) + F_{\pi,k}^h)(A_2^T J_k(t) + F_{\pi,k}^h) - \chi(A_3^T J_k(t) + F_{\pi,k}^h), \tag{40}$$

where

$$F_{\pi,k}^h = A^T J(t) - A^T J_k(t), \tag{41}$$

$$F_{D,k}^{\nu,h} = D^{(\nu)} J_k(t) - D^{\nu} J_k(t). \tag{42}$$

Residual for Eq (40) is

$$R_k^{(F)}(t) = A_1^T D^{(\nu)} Y_k(t) + F_{D,k}^{\nu,h} + \omega(A_1^T J_k(t) + F_{\pi,k}^h)(A_2^T J_k(t) + F_{\pi,k}^h) - \chi(A_3^T J_k(t) + F_{\pi,k}^h), \tag{43}$$

when Eq (43) is collocated at k points

$$t_r = \frac{r}{k}, \quad r = 0, 1, 2, \cdots, k-1,$$

we obtain

$$R_k^{(F)}(t_r) = A_1^T D^{(\nu)} Y_k(t_r) + F_{D,k}^{\nu,h} + \omega(A_1^T J_k(t_r) + F_{\pi,k}^h)(A_2^T Y_k(t_r) + F_{\pi,k}^h) - \chi(A_3^T J_k(t_r) + F_{\pi,k}^h). \tag{44}$$

Ultimately, Eqs (32) and (44) lead to a set of non-linear algebraic equations. We solve the system to find the value of the unknowns. Afterward, we move on to solving Eq (39). Let the achieved solution be represented by $\zeta_k^*(t)$.

Now, applying the limit $k \longrightarrow \infty$ and using Theorems 5.1 and 5.2, we get

$$\zeta_k^*(t) \longrightarrow \zeta_k(t). \tag{45}$$

From Eq (45) and Theorem 5.3, we get that

$$\lim_{k\to\infty} \zeta_k(t) = \zeta(t).$$

For FDEs (6)–(8), the same proof can be created. □

6. Overview of the VLCM method

Here, we will review the algorithm that uses the collocation approach and operational matrix to generate the fractional DE solution [32–35]. We utilize the subsequent approximation:

$$\psi(t) = \sum_{r=0}^{k} b_r v_r^{(p,q)}(t) = C^T V_k(t). \tag{46}$$

Next, by taking the derivative of (46) at order one, we arrive at

$$D'\psi(t) = C^T D' V_k(t) \cong C^T D^{(1)} V_k(t), \tag{47}$$

here $D^{(1)}$ denotes the operational differentiation matrix of order 1 for VLPs.

Taking order ν derivative of (46), we get

$$D^{\nu}\psi(t) = C^T D^{\nu} V_k(t) \cong C^T D^{(\nu)} V_k(t), \tag{48}$$

here $D^{(\nu)}$ denotes the operational differentiation matrix of order ν for VLPs.

From Eqs (46) and (47), we can write

$$\psi(0) = C^T V_k(0), \tag{49}$$

$$\psi'(0) = C^T D^{(1)} V_k(0). \tag{50}$$

7. Numerical simulation of the FMMER model by VLCM

Grouping Eqs (5), (46) and (48), we obtain

$$C_1^T D^{(\nu)} V_k(t) + \omega(C_1^T V_k(t))(C_2^T V_k(t)) - \chi(C_3^T V_k(t)) = 0. \tag{51}$$

Grouping Eqs (6), (46) and (48), we obtain

$$C_2^T D^{(\nu)} V_k(t) + \omega(C_1^T V_k(t))(C_2^T V_k(t)) - (\chi + \beta)(C_3^T V_k(t)) = 0. \tag{52}$$

Grouping Eqs (7), (46) and (48), we obtain

$$C_3^T D^{(\nu)} V_k(t) - \omega(C_1^T V_k(t))(C_2^T V_k(t)) + (\chi + \beta)(C_3^T V_k(t)) = 0. \tag{53}$$

Grouping Eqs (8), (46) and (48), we obtain

$$C_4^T D^{(\nu)} V_k(t) - \beta(C_3^T V_k(t)) = 0. \tag{54}$$

The residual for Eqs (51)–(54) are

$$R_{1k}(t) = C_1^T D^{(\nu)} V_k(t) + \omega(C_1^T V_k(t))(C_2^T V_k(t)) - \chi(C_3^T V_k(t)), \tag{55}$$

$$R_{2k}(t) = C_2^T D^{(\nu)} V_k(t) + \omega(C_1^T V_k(t))(C_2^T V_k(t)) - (\chi + \beta)(C_3^T V_k(t)), \tag{56}$$

$$R_{3k}(t) = C_3^T D^{(\nu)} V_k(t) - \omega(C_1^T V_k(t))(C_2^T V_k(t)) + (\chi + \beta)(C_3^T V_k(t)), \tag{57}$$

$$R_{4k}(t) = C_4^T D^{(\nu)} V_k(t) - \beta(C_3^T V_k(t)). \tag{58}$$

Now, when Eqs (55)–(58) are collocated at k points

$$t_r = \frac{r}{k}, \quad r = 0, 1, 2, \cdots, k-1,$$

we obtain

$$R_{1k}(t_r) = C_1^T D^{(\nu)} V_k(t_r) + \omega(C_1^T V_k(t_r))(C_2^T V_k(t_r)) - \chi(C_3^T V_k(t_r)), \tag{59}$$

$$R_{2k}(t_r) = C_2^T D^{(\nu)} V_k(t_r) + \omega(C_1^T V_k(t_r))(C_2^T V_k(t_r)) - (\chi + \beta)(C_3^T V_k(t_r)), \tag{60}$$

$$R_{3k}(t_r) = C_3^T D^{(\nu)} V_k(t_r) - \omega(C_1^T V_k(t_r))(C_2^T V_k(t_r)) + (\chi + \beta)(C_3^T V_k(t_r)), \tag{61}$$

$$R_{4k}(t_r) = C_4^T D^{(\nu)} V_k(t_r) - \beta(C_3^T V_k(t_r)). \tag{62}$$

Furthermore, from Eq (49), we get

$$C_1^T V_k(0) - \varepsilon(0) = 0, \tag{63}$$

$$C_2^T V_k(0) - \varphi(0) = 0, \tag{64}$$

$$C_3^T V_k(0) - \varrho(0) = 0, \tag{65}$$

$$C_4^T V_k(0) - \vartheta(0) = 0. \tag{66}$$

By using the collocation points in Eqs (59)–(62) along with Eqs (63)–(66), we are left with a non-linear system of equations that have the same amount of unknowns. The FMMER model's estimated solution is obtained by solving this system.

8. Analysis of the plan for VLCM

Theorem 8.1. Define the function as ψ: $[0, 1] \longrightarrow R$, $\psi \in C^{(k+1)}[0, 1]$. The k^{th} estimate found using VLPs is $\psi_k(z)$. Then,

$$E_{\psi,k}^f = \|\psi - \psi_k\|_{L_f^2[0,1]}, \tag{67}$$

and as $k \longrightarrow \infty$, the error vector $E_{\psi,k}^f \longrightarrow 0$.

Proof. For evidence, consult the relevant books [36, 37], and the study article [38]. □

Theorem 8.2. The error vector for ν order operational matrix differentiation is $E_{D,k}^{\nu,f}$, and it is computed utilizing $(k + 1)$ VLPs. Then,

$$E_{D,k}^{\nu,f} = D^{(\nu)} V_k(t) - D^{\nu} V_k(t), \tag{68}$$

and as $k \longrightarrow \infty$, $E_{D,k}^{\nu,f} \longrightarrow 0$.

Proof. [39, 40] are available for viewing. □

Theorem 8.3. Consider the functional U. Then

$$\lim_{k\to\infty} \gamma_k(t) = \gamma(t) = \inf_{t\in[0,1]} U(t). \tag{69}$$

Proof. See [41]. For Eq (5), the functional U is:

$$U(t) = D_t^{\gamma}\varepsilon(t) + \omega\varepsilon(t)\varphi(t) + \chi\varrho(t). \tag{70}$$

Using Eqs (46) and (48), we obtain

$$U^{(E)}(t) = C_1^T D^{(\nu)} U_k(t) + E_{D,k}^{\nu,f} + \omega(C_1^T V_k(t) + E_{\psi,k}^f)(C_2^T V_k(t) + E_{\psi,k}^f) - \chi(C_3^T V_k(t) + E_{\psi,k}^f), \tag{71}$$

where

$$E_{\psi,k}^f = C^T V(t) - C^T V_k(t), \tag{72}$$

$$E_{D,k}^{\nu,f} = D^{(\nu)} V_k(t) - D^{\nu} V_k(t). \tag{73}$$

Residual, for Eq (71) is

$$R_k^{(E)}(t) = C_1^T D^{(\nu)} U_k(t) + E_{D,k}^{\nu,f} + \omega(C_1^T V_k(t) + E_{\psi,k}^f)(C_2^T V_k(t) + E_{\psi,k}^f) - \chi(C_3^T V_k(t) + E_{\psi,k}^f), \quad (74)$$

when Eq (74) is collocated at k point

$$t_r = \frac{r}{k}, \quad r = 0, 1, 2, \cdots, k-1,$$

we obtain

$$R_k^{(E)}(t_r) = C_1^T D^{(\nu)} U_k(t_r) + E_{D,k}^{\nu,f} + \omega(C_1^T V_k(t_r) + E_{\psi,k}^f)(C_2^T V_k(t_r) + E_{\psi,k}^f) - \chi(C_3^T V_k(t_r) + E_{\psi,k}^f). \quad (75)$$

Ultimately, Eqs (63) and (75) lead to a set of non-linear algebraic equations. To determine the unknown values, we solve the system. Then we solve Eq (70). Let the achieved solution be represented by $\gamma_k^*(t)$.

Now, applying the limit $k \longrightarrow \infty$ and using Theorems 8.1 and 8.2,

$$\gamma_k^*(t) \longrightarrow \gamma_k(t). \quad (76)$$

From Eq (76) and Theorem 8.3, we get

$$\lim_{k\to\infty} \gamma_k(t) = \gamma(t).$$

For FDEs (6)–(8), the same proof can be created. □

9. Numerical results and discussion

Tables 1–4 compare the numerically calculated responses of $\varepsilon(t)$, $\varphi(t)$, $\varrho(t)$ and $\vartheta(t)$ using the collocation technique based-on shifted JPs and the collocation technique based on shifted VLPs.

Table 1. Comparison of numerical value of $\varepsilon(t)$ obtained by VLCM and JCM for $t = 0.01$ to 0.05 and $k = 4$.

t	$VLCM$	JCM
0.01	0.5387	0.5387
0.02	0.5757	0.5757
0.03	0.6111	0.6111
0.04	0.6450	0.6450
0.05	0.6774	0.6774

Table 2. Comparison of numerical value of $\varphi(t)$ obtained by VLCM and JCM for $t = 0.01$ to 0.05 and $k = 4$.

t	$VLCM$	JCM
0.01	0.1584	0.1584
0.02	0.2146	0.2146
0.03	0.2687	0.2687
0.04	0.3207	0.3207
0.05	0.3708	0.3708

Table 3. Comparison of numerical value of $\varrho(t)$ obtained by VLCM and JCM for $t = 0.01$ to 0.05 and $k = 4$.

t	$VLCM$	JCM
0.01	1.9416	1.9416
0.02	1.8854	1.8854
0.03	1.8313	1.8313
0.04	1.7793	1.7793
0.05	1.7292	1.7292

Table 4. Comparison of numerical value of $\vartheta(t)$ obtained by VLCM and JCM for $t = 0.01$ to 0.05 and $k = 4$.

t	$VLCM$	JCM
0.01	9.0197	9.0197
0.02	9.0389	9.0389
0.03	9.0576	9.0576
0.04	9.0757	9.0757
0.05	9.0934	9.0934

Numerical simulation and graphical results of the fractional order enzymatic reaction model are displayed in the Figures 1–4 which is obtained by JCM. Figures 1–4 present the behaviour of ε, φ, ϱ and ϑ, respectively, with time. $\varepsilon(t)$ exhibits a tendency to rise with respect to time, and the rate of increase, decreases when fractional order rises from 0.8 to 1 (see Figure 1). $\varphi(t)$ displays a tendency to increase with respect to time, and the rate of increase, decreases when fractional order is increased from 0.8 to 1 (see Figure 2). $\varrho(t)$ demonstrates a tendency to decline over time, and rate of decrese, increases as fractional order rises from 0.8 to 1 (see Figure 3). $\vartheta(t)$ indicates a tendency to increase with respect to time, and the rate of increase, decreases as fractional order rises from 0.8 to 1 (see Figure 4). Figures 5 and 6 show the comparison between JCM and VLCM.

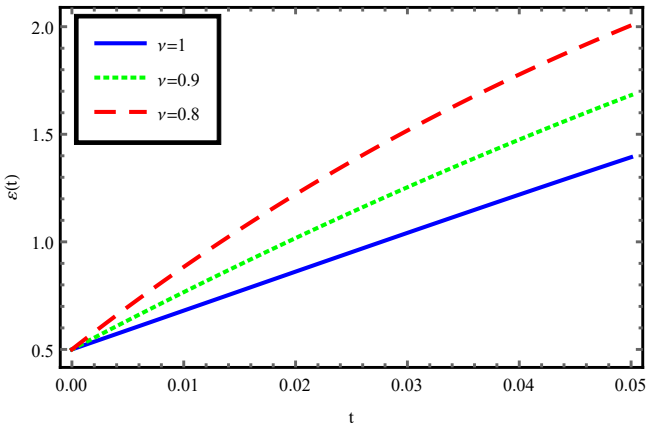


Figure 1. Graph of $\varepsilon(t)$ vs t at $p = 1$, $q = 1$, $k = 8$, $\varepsilon_0 = 0.5$, $\omega = 1$, $\beta = 1$ and $\chi = 2$.

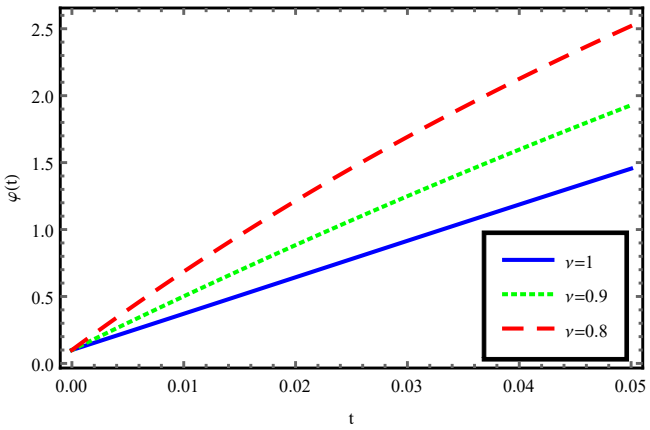


Figure 2. Graph of $\varphi(t)$ vs t at $p = 1$, $q = 1$, $k = 8$, $\varphi_0 = 0.1$, $\omega = 1$, $\beta = 1$ and $\chi = 2$.

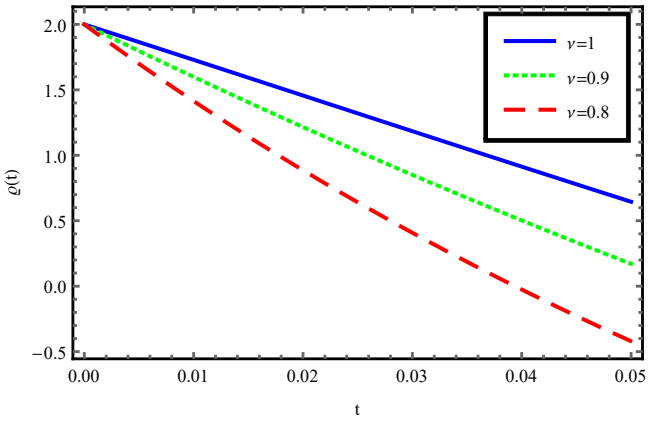


Figure 3. Graph of $\varrho(t)$ vs t at $p = 1$, $q = 1$, $k = 8$, $\varrho_0 = 2$, $\omega = 1$, $\beta = 1$ and $\chi = 2$.

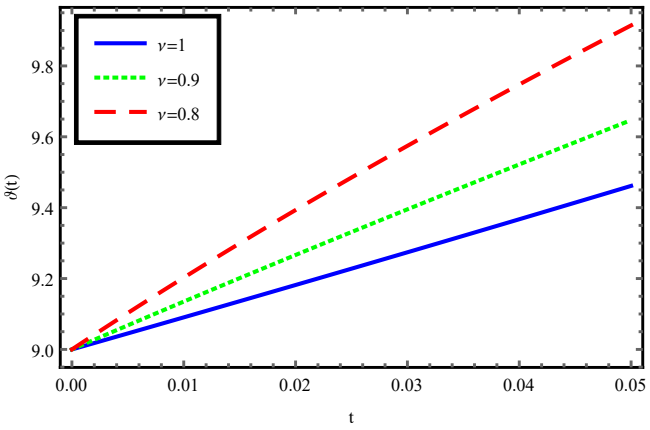
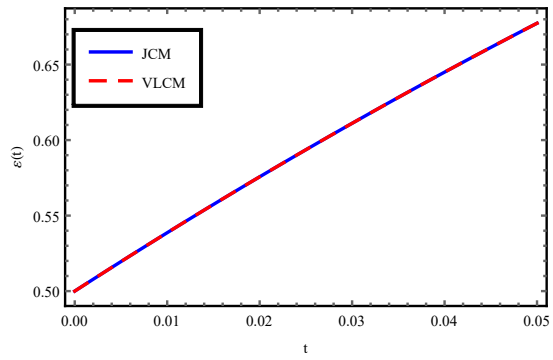
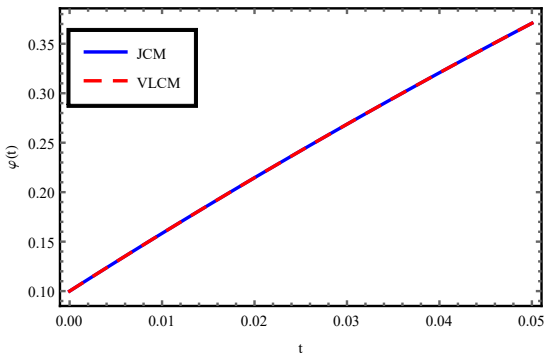


Figure 4. Graph of $\vartheta(t)$ vs t at $p = 1$, $q = 1$, $k = 8$, $\vartheta_0 = 9$, $\omega = 1$, $\beta = 1$ and $\chi = 2$.

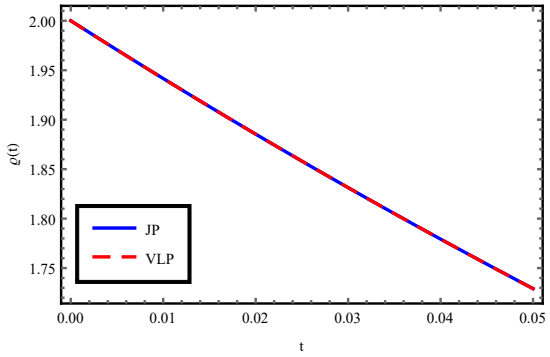


(a) Graph of $\varepsilon(t)$ vs t for $\nu = 1$ obtain by collocation technique using JPs and VLPs.

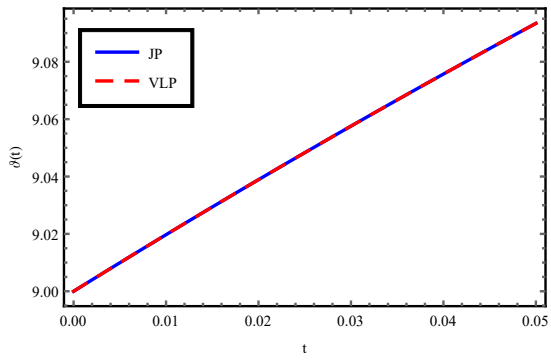


(b) Graph of $\varphi(t)$ vs t for $\nu = 1$ obtain by collocation technique using JPs and VLPs.

Figure 5. Comparison between JCM and VLCM.



(a) Graph of $\varrho(t)$ vs t for $\nu = 1$ obtain by collocation technique using JPs and VLPs.



(b) Graph of $\vartheta(t)$ vs t for $\nu = 1$ obtain by collocation technique using JPs and VLPs.

Figure 6. Comparison between JCM and VLCM.

10. Conclusions

To evaluate the computational solutions of the FMMER model, two computational techniques have been discussed in the present article. In this work, we present a novel operational matrix for derivatives of arbitrary order for JPs and VLPs in the Caputo sense. A computer-based mathematical algorithm is created using an operational matrix to resolve the nonlinear FDEs that contain the Caputo arbitrary order derivative. The benefit of using the proposed mathematical technique is that it reduces the issues to a simple set of algebraic equations that is solvable using any type of computing device. Algebraic equations are solved in this research study using Newton's approach. To compute numerical results, we use Mathematica computer software. The numerical results show the recommended approach's accuracy, success and trustworthiness. We found that our approach leds to more effective outcomes. The computer solution of the FMMER model using a collocation approch shows that this technique can be applied to explain chemical difficulties that occur in chemistry. We can solve more complex

fractional calculus problems using the collocation technique that arises in real words.

Use of AI tools declaration

The authors declare they have not used Artificial Intelligence (AI) tools in the creation of this article.

Conflict of interest

The authors declare no conflicts of interest in this manuscript.

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