

Analysis of variable-order Caputo fractional derivative for enzyme kinetics model

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Abstract Chemical kinetics explores the speed of chemical reactions and the various factors that govern their progression. It examines how reactant concentrations, temperature, catalysts, and reaction mechanisms affect reaction speed. The field provides essential insights into reaction pathways, helping in the design of efficient chemical processes in industries such as pharmaceuticals, energy, and environmental science. This work introduces a novel fractional variable-order model of enzyme kinetics, utilizing the Caputo derivative to capture complex kinetic behavior. The model is formulated using fractional variable-order differential equations, extending classical enzyme kinetics to better represent real-world enzymatic processes. We establish the existence and uniqueness of solutions for the enzyme kinetics model using fixed point theory. A numerical simulation is performed to approximate the solution dynamics. Our results demonstrate the value of Caputo fractional variable-order models in enzyme reaction kinetics, providing deeper insights into complex biochemical processes.

1 Introduction

Enzyme kinetics is fundamental to understanding chemical reaction mechanisms, especially in biochemical and industrial contexts. Mathematical modeling is essential for studying these reactions, providing a systematic approach to analyze mechanisms, predict behavior, and optimize processes. Because enzymatic reactions are complex, involving substrates, enzymes, and inhibitors, mathematical models are crucial for capturing the underlying kinetics that experimental methods alone may miss. These models describe substrate concentration changes and enzyme influence on reaction rates, enabling prediction and optimization. They also aid in estimating key parameters like reaction rate constants and inhibition effects. Mathematical models are particularly valuable for handling the complexity of real-world systems with multiple interacting components. The applications are vast, spanning pharmaceuticals and biotechnology, where enzyme kinetics modeling contributes to drug design, fermentation optimization, and enzyme-based manufacturing.

Classical enzyme kinetic models, like Michaelis-Menten and Briggs-Haldane, often fall short of capturing the intricate memory and hereditary characteristics observed in biochemical reactions [12, 13]. Fractional calculus offers a powerful alternative, enabling the development of more realistic models. Fractional-order models, incorporating non-locality and memory effects, better represent the real-world behavior of enzymatic reactions. Mathematical models of enzyme kinetics incorporating different fractional-order derivatives have been extensively studied using numerous methods (see references, [11, 14, 15, 16, 17] and therein).

The study of variable-order Caputo fractional derivatives (VOCFD) is essential in a wide range of real-world disciplines because many natural and engineered systems exhibit time-dependent dynamics, memory effects, and non-uniform behavior that traditional integer-order

models fail to capture. The key distinction between fixed-order and VOCFD lies in their treatment of memory effects. Fixed-order derivatives assume these effects are constant, while variable-order derivatives allow them to evolve, leading to more adaptable and realistic models [8, 19]. In biological systems, such as enzyme kinetics and disease modeling, reaction rates and diffusion properties often evolve over time, necessitating variable-order modeling for accurate predictions. In engineering and material sciences, processes like viscoelasticity, heat conduction, and fluid flow in porous media require flexible models to account for material aging and structural changes. Similarly, in control systems and signal processing, adaptive algorithms based on variable-order derivatives improve system stability and efficiency in real-time applications (see [7, 9, 10, 20]). By studying fractional variable-order derivatives, researchers gain a more comprehensive and realistic understanding of dynamic processes, leading to improved models, better predictions, and optimized solutions across multiple scientific and industrial fields. Recently, various dynamical systems have been developed in the context of fractional variable-order derivatives, as referenced in [1, 2, 3, 4, 5, 6, 18].

1.1 Motivation and contributions of the proposed work

The VOCFD is a powerful tool for studying enzyme kinetics, as it allows for a more flexible and accurate representation of reaction dynamics by incorporating memory effects and time-dependent behavior. Unlike traditional integer-order models, which assume a constant rate of change, the variable-order fractional derivative adapts dynamically, reflecting changes in enzyme activity and substrate interactions over time. This approach is particularly useful in biochemical reactions where reaction rates may vary due to environmental factors, enzyme inhibition, or substrate depletion. By integrating the Caputo variable-order derivative into enzyme kinetics models, researchers can better capture complex reaction mechanisms, predict anomalous diffusion behavior, and optimize biotechnological and pharmaceutical processes with greater precision.

Motivated by the aforementioned significance and broad applicability of variable-order fractional derivatives, we extend a model in [17] to a variable-order fractional derivative under Caputo sense. This study presents the following significant contributions:

- A VOCFD model for enzyme kinetics has been proposed.
- Establish the existence and uniqueness theory for the considered model using the fixed point theorems.
- Numerical simulations were conducted by employing the variable-order fractional Runge–Kutta method of fourth order (VOFRK4M), to solve the VOCFD model for enzyme kinetics.

1.2 Structure of the paper

The structure of this paper is as follows: A VOCFDM for enzyme kinetics is presented, in Sect 2. In Sect 3, positivity and boundness of the system is determined, existence and uniqueness results are discussed in Sect 4. In Sect 5, numerical methods for simulations and discussions are presented. Finally, Sect 6 concludes the manuscript.

2 Description of VOCFD model for enzyme kinetics

To analyze the mathematical model in order to investigate with the existence of solutions in an enzyme kinetics model using the information from the research that were previously discussed. The quantitative study of enzyme kinetics examines how enzyme activity varies in response to different substrate concentrations, reaction conditions, and other variables, as seen in [17]. The given conditions in the proposed system are independent of one another and satisfy $\mathbb{N}(t) = \mathbb{S}(t) + \mathbb{E}(t) + \mathbb{H}(t) + \mathbb{P}(t)$. The \mathbb{N} value represents the terms presented in the relevant system of reactions. The concentration of a substance is represented by square brackets [] and $[\mathbb{S}] = \mathbb{S}$, $[\mathbb{E}] = \mathbb{E}$, and $[\mathbb{H}] = \mathbb{H}$ as follows:

$$\begin{cases} \frac{d\mathbb{S}}{dt} = \beta_2\mathbb{H} - \beta_1\mathbb{E}, \\ \frac{d\mathbb{E}}{dt} = \beta_3\mathbb{H} + \beta_2\mathbb{H} - \beta_1\mathbb{E}\mathbb{S}, \\ \frac{d\mathbb{H}}{dt} = -\beta_3\mathbb{H} - \beta_2\mathbb{H} + \beta_1\mathbb{E}\mathbb{S}, \\ \frac{d\mathbb{P}}{dt} = \beta_3\mathbb{P}. \end{cases}$$

Examine the variable order Caputo fractional derivative in the enzyme kinetics and studing existence, uniqueness, and numerical simulations into account. The VOCFD model for enzyme kinetics is

$$\begin{cases} {}^C D^{\delta(t)}\mathbb{S}(t) = \beta_2\mathbb{H} - \beta_1\mathbb{E}\mathbb{S}, \\ {}^C D^{\delta(t)}\mathbb{E}(t) = \beta_3\mathbb{H} + \beta_2\mathbb{H} - \beta_1\mathbb{E}\mathbb{S}, \\ {}^C D^{\delta(t)}\mathbb{H}(t) = -\beta_3\mathbb{H} - \beta_2\mathbb{H} + \beta_1\mathbb{E}\mathbb{S}, \\ {}^C D^{\delta(t)}\mathbb{P}(t) = \beta_3\mathbb{P}. \end{cases} \tag{2.1}$$

With the initial condition, the enzyme kinetics model’s impact becomes $\mathbb{S}(0) = \mathbb{S}_0, \mathbb{E}(0) = \mathbb{E}_0, \mathbb{H}(0) = \mathbb{H}_0, \mathbb{P}(0) = \mathbb{P}_0$. Here, ${}^C D^{\delta(t)}$ denotes the variable-order Caputo fractional derivative of order $\delta(t)$, for $\delta(t) \in (0, 1]$. When one molecule of enzyme \mathbb{E} is combined with one molecule of substrate \mathbb{S} , an enzyme substrate \mathbb{H} composed of one molecule and the product \mathbb{P} are created, as can be seen when examining the chemical reaction (2.1). Here, β_1 is the rate at which enzymes develop, β_2 denotes the rate at which products are created, and β_3 denotes catalysis. Classical integer-order models, which are based on memoryless kinetics, often fail to capture the subtle time-dependent behaviors observed in real systems. In contrast, the variable-order fractional framework incorporates evolving memory effects, offering a more flexible and accurate description of reaction dynamics. This enhanced capability not only improves the predictive power of the models but also supports the development of more effective control strategies for complex industrial processes. The basic definitons and some results are detailed in the reference [3].

3 Positivity and Boundedness of the solution

Here, we demonstrate that the model (2.1) has the boundedness and positivity.

Theorem 3.1. *The solutions to the model (2.1) has the positivity property.*

Proof. From model (2.1), we have

$$\begin{cases} \mathbb{S}(t)|_{\mathbb{S}=0} = \beta_2\mathbb{H} - \beta_1\mathbb{E}\mathbb{S} > 0, \\ \mathbb{E}(t)|_{\mathbb{E}=0} = \beta_3\mathbb{H} + \beta_2\mathbb{H} - \beta_1\mathbb{E}\mathbb{S} > 0, \\ \mathbb{H}(t)|_{\mathbb{H}=0} = -\beta_3\mathbb{H} - \beta_2\mathbb{H} + \beta_1\mathbb{E}\mathbb{S} > 0, \\ \mathbb{P}(t)|_{\mathbb{P}=0} = \beta_3\mathbb{P}. \end{cases} \tag{3.1}$$

The outcome shows that none of the model’s parameters or reactions are negative. The proof can be effectively concluded since all solutions for our model (2.1) are guaranteed to be non-negativity. □

Theorem 3.2. *The solution of our model (2.1), denoted as*

$$Y = \left\{ \mathbb{S}(t), \mathbb{E}(t), \mathbb{H}(t), \mathbb{P}(t) \in \mathbb{R}^4 : 0 < \mathbb{N} \leq \frac{\varphi}{\rho} \right\}$$

, adheres to this invariant. The solution remains bounded within the positive invariant region \mathbb{R}^4 while considering initial conditions of $\mathbb{S} > 0, \mathbb{E} > 0, \mathbb{H} \geq 0$, and $\mathbb{P} \geq 0$.

Proof. Assume that $\mathbb{N}(t) = \mathbb{S}(t) + \mathbb{E}(t) + \mathbb{H}(t) + \mathbb{P}(t)$ and sum of the model (2.1), we get

$$\mathbb{N}(t) = \varphi - \rho\mathbb{N}, \tag{3.2}$$

then integrating Eq. 3.2, we obtain $Y = \left\{ \mathbb{S}(t) + \mathbb{E}(t) + \mathbb{H}(t) + \mathbb{P}(t) \leq \frac{y}{\varrho} \right\}$.

When t becomes very large i.e., $t \rightarrow \infty$, it implies that $\frac{y}{\varrho}$ is the supremum of \mathbb{N} , making it a positive invariant for the model (2.1). □

Remark. The assumptions in Theorem 3.2 serve two distinct purposes. The first set of assumptions specifies the initial conditions, ensuring that each compartment starts with biologically meaningful, non-negative values: $\mathbb{S}(0) > 0, \mathbb{E}(0) > 0, \mathbb{H}(0) \geq 0, \mathbb{P}(0) \geq 0$. The second assumption restricts the total population, $\mathbb{N}(t) = \mathbb{S}(t) + \mathbb{E}(t) + \mathbb{H}(t) + \mathbb{P}(t) \leq \frac{y}{\varrho}$, guaranteeing that the solution remains bounded within the positive invariant region. Together, these assumptions ensure that the model solutions are both biologically feasible and mathematically well-posed.

4 Existence and uniqueness results

In this setting, we use a fixed-point method to investigate whether a solution existence and is unique. To make it simpler, with the assumption (\mathcal{H}) :, we take into consideration the following hypothesis: For the $\mathbb{S}(t), \hat{\mathbb{S}}(t), \mathbb{E}, \hat{\mathbb{E}}(t), \mathbb{H}(t), \hat{\mathbb{H}}(t), \mathbb{P}(t)$ and $\hat{\mathbb{P}}(t) \in L[0, 1]$ be continuous function, such that $\|\mathbb{S}\| \leq b_1, \|\mathbb{E}\| \leq b_2, \|\mathbb{H}\| \leq b_3, \|\mathbb{P}\| \leq b_4$ for non-negative constant $b_1, b_2, b_3, b_4 > 0$. Further more we define the following constants: $\Phi_1 = \beta_1 b_2, \Phi_2 = \beta_1 b_1, \Phi_3 = \beta_3 + \beta_2, \Phi_4 = \beta_3$.

Theorem 4.1. *The kernels \mathcal{L}_j , for $j = 1, 2, 3, 4$ holds on Lipschitz condition, if the assumption (\mathcal{H}) is satisfied and $\Phi_j < 1$ for $j = 1, 2, 3, 4$.*

Proof. By using successive iterative technique, we apply the VOF integral representation to the suggested model (2.1).

$$\begin{cases} \mathbb{S}(t) = \mathbb{S}(0) + \frac{1}{\Gamma(\delta(t))} \int_0^t (t-v)^{\delta(t)-1} [\beta_2 \mathbb{H} - \beta_1 \mathbb{E} \mathbb{S}] dv \\ \mathbb{E}(t) = \mathbb{E}(0) + \frac{1}{\Gamma(\delta(t))} \int_0^t (t-v)^{\delta(t)-1} [\beta_3 \mathbb{H} + \beta_2 \mathbb{H} - \beta_1 \mathbb{E} \mathbb{S}] dv \\ \mathbb{H}(t) = \mathbb{H}(0) + \frac{1}{\Gamma(\delta(t))} \int_0^t (t-v)^{\delta(t)-1} [-\beta_3 \mathbb{H} - \beta_2 \mathbb{H} + \beta_1 \mathbb{E} \mathbb{S}] dv \\ \mathbb{P}(t) = \mathbb{P}(0) + \frac{1}{\Gamma(\delta(t))} \int_0^t (t-v)^{\delta(t)-1} [\beta_3 \mathbb{P}] dv. \end{cases} \tag{4.1}$$

Setting \mathcal{L}_j for $j = 1, 2, 3, 4$, then we have

$$\begin{cases} \mathcal{L}_1(t, \mathbb{S}) &= \beta_2 \mathbb{H} - \beta_1 \mathbb{E} \mathbb{S} \\ \mathcal{L}_2(t, \mathbb{E}) &= \beta_3 \mathbb{H} + \beta_2 \mathbb{H} - \beta_1 \mathbb{E} \mathbb{S} \\ \mathcal{L}_3(t, \mathbb{H}) &= -\beta_3 \mathbb{H} - \beta_2 \mathbb{H} + \beta_1 \mathbb{E} \mathbb{S} \\ \mathcal{L}_4(t, \mathbb{P}) &= \beta_3 \mathbb{P}. \end{cases} \tag{4.2}$$

The desired result is attained through assumption (\mathcal{H}) holds, and similarly with analogous reasoning for $\mathcal{L}_1(t, \mathbb{S})$ using the Lipschitz condition, we obtain:

$$\begin{aligned} \left\| \mathcal{L}_1(\mathbb{S}) - \mathcal{L}_1(\hat{\mathbb{S}}) \right\| &= \left\| [\beta_2 \mathbb{H} - \beta_1 \mathbb{E} \mathbb{S}] - [\beta_2 \mathbb{H} - \beta_1 \mathbb{E} \hat{\mathbb{S}}] \right\|, \\ &\leq \beta_1 \|\mathbb{S} - \hat{\mathbb{S}}\| \|\mathbb{E}\| = \Phi_1 \|\mathbb{S} - \hat{\mathbb{S}}\| \end{aligned}$$

this shows that $\Phi_1 = \beta_1 b_2$. As a result, \mathcal{L}_1 conforms to the Lipschitz condition, possessing a Lipschitz constant Φ_1 . Likewise, the remaining kernels also satisfy the Lipschitz condition.

$$\begin{aligned} \left\| \mathcal{L}_2(\mathbb{E}) - \mathcal{L}_2(\hat{\mathbb{E}}) \right\| &= \left\| [\beta_3 \mathbb{H} + \beta_2 \mathbb{H} - \beta_1 \mathbb{E} \mathbb{S}] - [\beta_3 \mathbb{H} + \beta_2 \mathbb{H} - \beta_1 \hat{\mathbb{E}} \mathbb{S}] \right\|, \\ &\leq \beta_1 \|\mathbb{E} - \hat{\mathbb{E}}\| \|\mathbb{S}\| = \Phi_2 \|\mathbb{E} - \hat{\mathbb{E}}\|, \end{aligned}$$

where $\Phi_2 = \beta_1 b_1$. Hence, \mathcal{L}_2 satisfies the Lipschitz condition with constant Φ_2 . Then

$$\begin{aligned} \left\| \mathcal{L}_3(\mathbb{H}) - \mathcal{L}_3(\hat{\mathbb{H}}) \right\| &= \left\| [-\beta_3 \mathbb{H} - \beta_2 \mathbb{H} + \beta_1 \mathbb{E} \mathbb{S}] - [-\beta_3 \hat{\mathbb{H}} - \beta_2 \hat{\mathbb{H}} + \beta_1 \mathbb{E} \mathbb{S}] \right\|, \\ &\leq (\beta_3 + \beta_2) \|\mathbb{H} - \hat{\mathbb{H}}\| = \Phi_3 \|\mathbb{H} - \hat{\mathbb{H}}\|, \end{aligned}$$

where $\Phi_3 = \beta_3 + \beta_2$. Hence, \mathcal{L}_3 satisfies the Lipschitz condition with constant Φ_3 . Then

$$\left\| \mathcal{L}_4(\mathbb{P}) - \mathcal{L}_4(\hat{\mathbb{P}}) \right\| = \left\| [\beta_3 \mathbb{P}] - [\beta_3 \hat{\mathbb{P}}] \right\|, \leq \beta_3 \|\mathbb{P} - \hat{\mathbb{P}}\| = \Phi_4 \|\mathbb{P} - \hat{\mathbb{P}}\|,$$

where $\Phi_4 = \beta_3$. Hence, \mathcal{L}_3 satisfies the Lipschitz condition with constant Φ_4 . Now, from Eq. (4.1), all the kernels \mathcal{L}_j , where $j = 1, 2, 3, 4$, satisfy the Lipschitz property, and the result can accomplish

$$\begin{cases} \mathbb{S}(t) = \mathbb{S}(0) + \frac{1}{\Gamma(\delta(t))} \int_0^t (t-v)^{\delta(t)-1} \mathcal{L}_1(v, \mathbb{S}(v)) dv \\ \mathbb{E}(t) = \mathbb{E}(0) + \frac{1}{\Gamma(\delta(t))} \int_0^t (t-v)^{\delta(t)-1} \mathcal{L}_2(v, \mathbb{E}(v)) dv \\ \mathbb{H}(t) = \mathbb{H}(0) + \frac{1}{\Gamma(\delta(t))} \int_0^t (t-v)^{\delta(t)-1} \mathcal{L}_3(v, \mathbb{H}(v)) dv \\ \mathbb{P}(t) = \mathbb{P}(0) + \frac{1}{\Gamma(\delta(t))} \int_0^t (t-v)^{\delta(t)-1} \mathcal{L}_4(v, \mathbb{P}(v)) dv. \end{cases}$$

□

Theorem 4.2. For the variable order Caputo fractional model (2.1) has a solution under assumption (H) then

$$\zeta = \max [\Phi_1, \Phi_2, \Phi_3, \Phi_4] < 1.$$

Proof. Let us define the four functions $\omega_{1\kappa}, \omega_{2\kappa}, \omega_{3\kappa}$, and $\omega_{4\kappa}$ by employing a sequential iterative technique (2.1) as follows,

$$\begin{cases} \omega_{1\kappa}(t) = \mathbb{S}_{\kappa+1}(t) - \mathbb{S}(t), \omega_{2\kappa}(t) = \mathbb{E}_{\kappa+1}(t) - \mathbb{E}(t), \\ \omega_{3\kappa}(t) = \mathbb{H}_{\kappa+1}(t) - \mathbb{H}(t), \omega_{4\kappa}(t) = \mathbb{P}_{\kappa+1}(t) - \mathbb{P}(t). \end{cases} \tag{4.3}$$

Then, we have

$$\begin{cases} \|\omega_{1\kappa}(t)\| &= \frac{1}{\Gamma(\delta(t))} \int_0^t (t-v)^{\delta(t)-1} \|\mathcal{L}_1(v, \mathbb{S}_\kappa(v)) - \mathcal{L}_1(v, \mathbb{S}_\kappa(v))\| dv \\ &\leq \frac{t^{\delta(t)}}{\Gamma(\delta(t)+1)} \Phi_1 \|\mathbb{S}_\kappa - \mathbb{S}\| \\ &\leq \frac{t^{\delta(t)}}{\Gamma(\delta(t)+1)} \Phi_1^\kappa \|\mathbb{S}_1 - \mathbb{S}\|. \end{cases} \tag{4.4}$$

According that, we can estimate

$$\begin{cases} \|\omega_{2\kappa}(t)\| &= \frac{1}{\Gamma(\delta(t))} \int_0^t (t-v)^{\delta(t)-1} \|\mathcal{L}_2(v, \mathbb{E}_\kappa(v)) - \mathcal{L}_2(v, \mathbb{E}_\kappa(v))\| dv \\ &\leq \frac{t^{\delta(t)}}{\Gamma(\delta(t)+1)} \Phi_2 \|\mathbb{E}_\kappa - \mathbb{E}\| \\ &\leq \left[\frac{t^{\delta(t)}}{\Gamma(\delta(t)+1)} \right]^\kappa \Phi_2^\kappa \|\mathbb{E}_1 - \mathbb{E}\|. \end{cases} \tag{4.5}$$

$$\begin{cases} \|\omega_{3\kappa}(t)\| &= \frac{1}{\Gamma(\delta(t))} \int_0^t (t-v)^{\delta(t)-1} \|\mathcal{L}_3(v, \mathbb{H}_\kappa(v)) - \mathcal{L}_3(v, \mathbb{H}_\kappa(v))\| dv \\ &\leq \frac{t^{\delta(t)}}{\Gamma(\delta(t)+1)} \Phi_3 \|\mathbb{H}_\kappa - \mathbb{H}\| \\ &\leq \left[\frac{t^{\delta(t)}}{\Gamma(\delta(t)+1)} \right]^\kappa \Phi_3^\kappa \|\mathbb{H}_1 - \mathbb{H}\|. \end{cases} \tag{4.6}$$

Finally, we obtain

$$\begin{cases} \|\omega_{4\kappa}(t)\| &= \frac{1}{\Gamma(\delta(t))} \int_0^t (t-v)^{\delta(t)-1} \|\mathcal{L}_4(v, \mathbb{P}_\kappa(v)) - \mathcal{L}_4(v, \mathbb{P}_\kappa(v))\| dv \\ &\leq \frac{t^{\delta(t)}}{\Gamma(\delta(t)+1)} \Phi_4 \|\mathbb{P}_\kappa - \mathbb{P}\| \\ &\leq \left[\frac{t^{\delta(t)}}{\Gamma(\delta(t)+1)} \right]^\kappa \Phi_4^\kappa \|\mathbb{P}_1 - \mathbb{P}\|. \end{cases} \tag{4.7}$$

By Eqs. (4.4)-(4.7), taking the limit on both sides as $\kappa \rightarrow \infty$, the functions mentioned above exhibit the property of $\omega_{j\kappa}(t) \rightarrow 0$ for $j = 1, 2, 3, 4$, given that $\Phi_j < 1, (j = 1, 2, 3, 4)$. We conclude the model (2.1) has a solution, which completes the proof. □

Theorem 4.3. The variable order Caputo fractional model (2.1) admits unique solution if the assumption (H) satisfied and $\frac{t^{\delta(t)}}{\Gamma(\delta(t)+1)} \Phi_j \leq 1$, for $j \in \mathcal{N}_1^4$.

Proof. Let us consider that the another existing solution $(\hat{\mathbb{S}}, \hat{\mathbb{E}}, \hat{\mathbb{H}}, \hat{\mathbb{P}})$ with initial values $(\hat{\mathbb{S}}(0), \hat{\mathbb{E}}(0), \hat{\mathbb{H}}(0), \hat{\mathbb{P}}(0))$ we have

$$\hat{\mathbb{S}}(t) = \hat{\mathbb{S}}(0) + \frac{1}{\Gamma(\delta(t))} \int_0^t (t-v)^{\delta(t)-1} \mathcal{L}_1(v, \hat{\mathbb{S}}(v)) dv$$

then, follows as

$$\hat{\mathbb{E}}(t) = \hat{\mathbb{E}}(0) + \frac{1}{\Gamma(\delta(t))} \int_0^t (t-v)^{\delta(t)-1} \mathcal{L}_2(v, \hat{\mathbb{E}}(v)) dv$$

$$\hat{\mathbb{H}}(t) = \hat{\mathbb{H}}(0) + \frac{1}{\Gamma(\delta(t))} \int_0^t (t-v)^{\delta(t)-1} \mathcal{L}_3(v, \hat{\mathbb{H}}(v)) dv$$

$$\hat{\mathbb{P}}(t) = \hat{\mathbb{P}}(0) + \frac{1}{\Gamma(\delta(t))} \int_0^t (t-v)^{\delta(t)-1} \mathcal{L}_4(v, \hat{\mathbb{P}}(v)) dv.$$

Again we have,

$$\begin{aligned} |\mathbb{S} - \hat{\mathbb{S}}| &= \frac{1}{\Gamma(\delta(t))} \int_0^t (s-v)^{\delta(t)-1} \left\| \mathcal{L}_1(v, \hat{\mathbb{E}}(v)) - \mathcal{L}_1(v, \mathbb{E}(v)) \right\| dv \\ &\leq \frac{1}{\Gamma(\delta(t))} \int_0^t (s-v)^{\delta(t)-1} \Phi_1 \left\| \mathbb{S}_1 - \hat{\mathbb{S}} \right\| \\ &\leq \frac{s^{\delta(t)}}{\Gamma(\delta(t) + 1)} \Phi_1 \left\| \mathbb{S}_1 - \hat{\mathbb{S}} \right\|. \end{aligned}$$

Then, we have

$$\frac{s^{\delta(t)}}{\Gamma(\delta(t) + 1)} \Phi_1 \left\| \mathbb{S}_1 - \hat{\mathbb{S}} \right\| \leq 0. \tag{4.8}$$

The inequality (4.8) mentioned above holds true in the case where $\|\mathbb{S} - \hat{\mathbb{S}}\| = 0$. This subsequently leads to the conclusion that $\mathbb{S} = \hat{\mathbb{S}}$, thereby establishing the uniqueness of the solution. The same results also exist for $\mathbb{E}, \mathbb{H},$ and \mathbb{P} . Thus, it can be concluded that a unique solution is admitted by the model (2.1). \square

5 Numerical analysis for variable order Caputo derivative

In this section, we present VOFRK4M algorithm as follows. Let us define the general structure of variable order Caputo fractional differential equation:

$$\begin{aligned} {}^C D^{\delta(t)} x(t) &= f(t, x(t)), \quad 0 < \delta(t) \leq 1, t \in [a, b], \\ x(0) &= x_0 \end{aligned}$$

The approximation solution can be obtain for the expansion

$$x_{n+1} = x_n + \frac{h^{\delta(t)}}{6\Gamma(\delta(t) + 1)} (K_1 + 2K_2 + 2K_3 + K_4),$$

where K_1, \dots, K_4 are functions.

$$\begin{aligned} K_1 &= f(t_n, x_n), \\ K_2 &= f\left(t_n + \frac{1}{2} \frac{h^{\delta(t)}}{\Gamma(\delta(t) + 1)}, \quad x_n + \frac{1}{2} \frac{h^{\delta(t)}}{\Gamma(\delta(t) + 1)} K_1\right), \\ K_3 &= f\left(t_n + \frac{1}{2} \frac{h^{\delta(t)}}{\Gamma(\delta(t) + 1)}, \quad x_n + \frac{1}{2} \frac{h^{\delta(t)}}{\Gamma(\delta(t) + 1)} K_2\right), \\ K_4 &= f\left(t_n + \frac{h^{\delta(t)}}{\Gamma(\delta(t) + 1)}, \quad x_n + \frac{h^{\delta(t)}}{\Gamma(\delta(t) + 1)} K_3\right). \end{aligned}$$

Algorithm 1 VOFRK4M

- Step 1:** Define $\delta(t)$, N , $t_0 = a$, $t_f = b$, $h = 0.01$, $N = \frac{t_f - t_0}{h}$.
- Step 2:** Define a state equations $x(t)$.
- Step 3:** Consider the initial conditions x_0 .
- Step 4:** for $i = 2, 3, \dots, N + 1$, to calculate the approximation solution x_2, x_3, \dots, x_{N+1} .
- Step 5:** for $i=2:N+1$
 - To find K_1, K_2, K_3, K_4 .
 - Substitute above values in x_n ,
 - we get the approximation values.
- end**
- Step 6:** Plot the above values with respect to time $[a, b]$ on various $\delta(t)$ and step size N .

5.1 VOFRK4M for enzyme kinetics model

For numerical solution of suggested variable-order enzyme kinetics system with arbitrary-order Caputo derivative, we utilize the above proposed VOFRK4M. In view of proposed numerical scheme the proposed model can be discretized as follows:

$$\begin{aligned}
 S_{n+1} &= S_n + \frac{h^{\delta(t)}}{6\Gamma(\delta(t) + 1)} (K_1 + 2K_2 + 2K_3 + K_4), \\
 E_{n+1} &= E_n + \frac{h^{\delta(t)}}{6\Gamma(\delta(t) + 1)} (K_1 + 2K_2 + 2K_3 + K_4), \\
 H_{n+1} &= H_n + \frac{h^{\delta(t)}}{6\Gamma(\delta(t) + 1)} (K_1 + 2K_2 + 2K_3 + K_4), \\
 P_{n+1} &= P_n + \frac{h^{\delta(t)}}{6\Gamma(\delta(t) + 1)} (K_1 + 2K_2 + 2K_3 + K_4),
 \end{aligned}$$

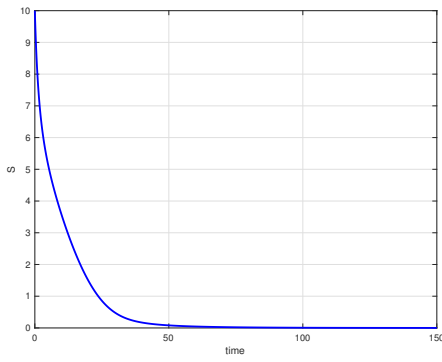
where $A = \frac{1}{2} \frac{h^{\delta(t)}}{\Gamma(\delta(t)+1)}$, $B = \frac{h^{\delta(t)}}{\Gamma(\delta(t)+1)}$

$$\begin{aligned}
 K_1 &= f(t_n, S_n, E_n, H_n, P_n), \\
 K_2 &= f(t_n + A, S_n + AK_1, E_n + AK_1, H_n + AK_1, P_n + AK_1), \\
 K_3 &= f(t_n + A, S_n + AK_2, E_n + AK_2, H_n + AK_2, P_n + AK_2), \\
 K_4 &= f(t_n + B, S_n + BK_3, E_n + BK_3, H_n + BK_3, P_n + BK_3).
 \end{aligned}$$

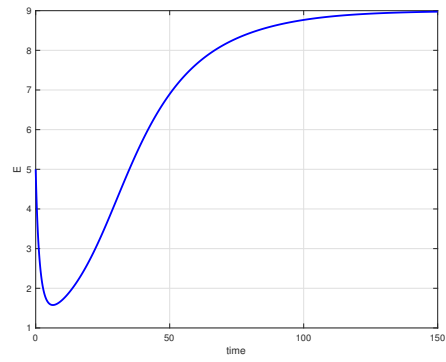
5.2 Discussion

In this section, we discuss a numerical approach aimed at solving the variable order Caputo enzyme kinetics model. Here, we consider the VOFRK4M order method for solving this model for $t = 100$ and $0 < \delta(t) \leq 1$ with initial conditions $S(0) = 10$, $E(0) = 5$, $H(0) = 4$, and $P(0) = 0.1$. The system parameter values $\beta_1 = 0.0530$ $\beta_2 = 0.012$, $\beta_3 = 0.040$.

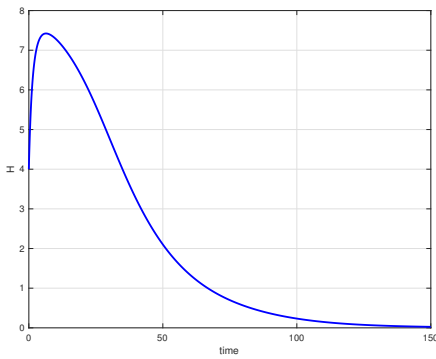
In Figure 1 represents the variable order enzyme kinetics model for Caputo fractional derivative with order $\delta(t) = 0.95 + 0.01 \sin(t/10)$. In Figure 1a presents the time response of concentration of substrate. In Figure 1b presents the time response of concentration of enzyme. In Figure 1c presents the time response of concentration of enzyme–substrate complex. In Figure 1d presents the time response of concentration of product.



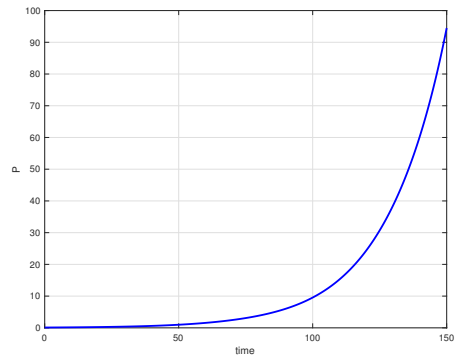
(a) Time response S



(b) Time response of E



(c) Time response of H



(d) Time response P

Figure 1: Time responses of Variable order Enzyme model with $\delta(t) = 0.95 + 0.01 \sin(t/10)$

Figure 2 represents the distinct variable-order enzyme kinetics model for the Caputo fractional derivative, with orders $\delta(t) = 0.98 + 0.008 \cos(t/10)$, $\delta(t) = 0.95 + 0.001 \sin(t/10)$ and $\delta(t) = 0.94 - (0.01/100)t$ respectively. In Figure 2a presents the time response of concentration of substrate. In Figure 2b presents the time response of concentration of enzyme. In Figure 2c presents the time response of concentration of enzyme–substrate complex. In Figure 2d presents the time response of concentration of product.

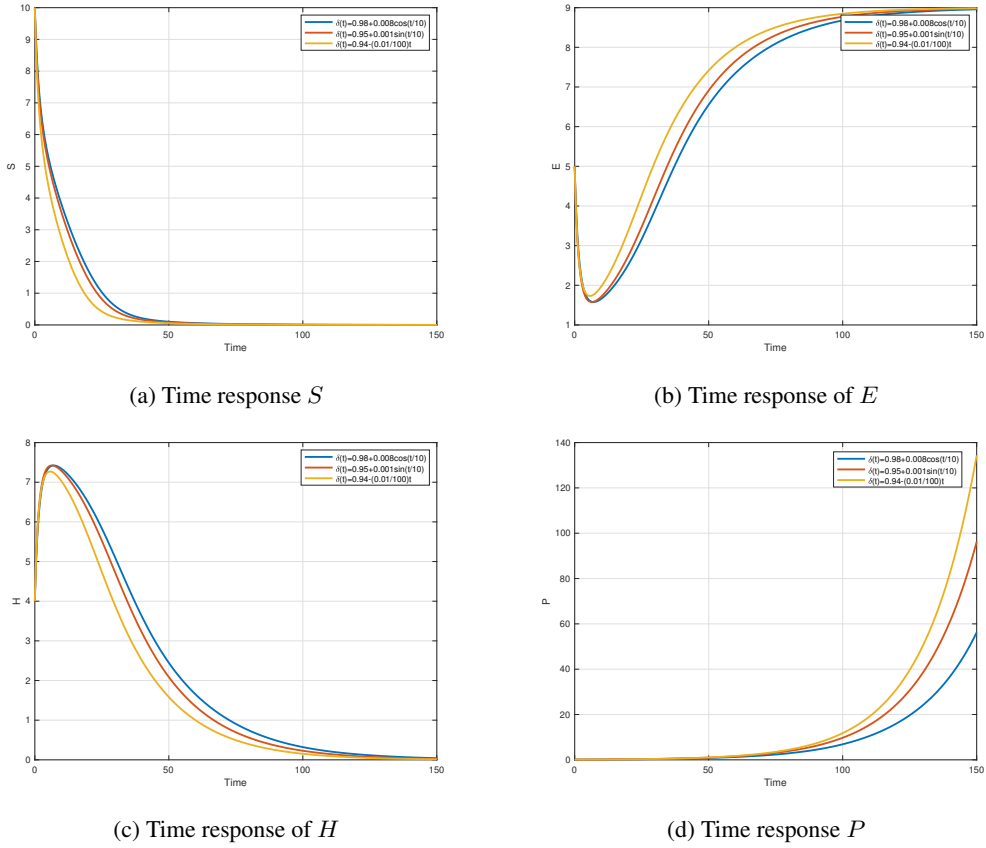


Figure 2: Time responses of distinct variable order Enzyme model

In Figure 3 represents the comparison analysis of integer, fractional and variable order enzyme kinetics model for Caputo fractional derivative with order $\delta(t) = 1$, $\delta(t) = 0.96$ and $\delta(t) = 0.94 - (0.01/100)t$ respectively. In Figure 3a presents the time response of concentration of substrate. In Figure 3b presents the time response of concentration of enzyme. In Figure 3c presents the time response of concentration of enzyme–substrate complex. In Figure 3d presents the time response of concentration of product.

Significant differences in system dynamics emerge when the model (2.1) is analyzed graphically under integer, fractional, and variable order derivative . From Figure 3, we conclude that the VOFRK4M is more accurate compared to classical and fractional-order systems, as it balances reaction speed, memory effects, and adaptability to different conditions. Additionally, its ability to enhance reaction speed allows for increased product formation in a shorter time.

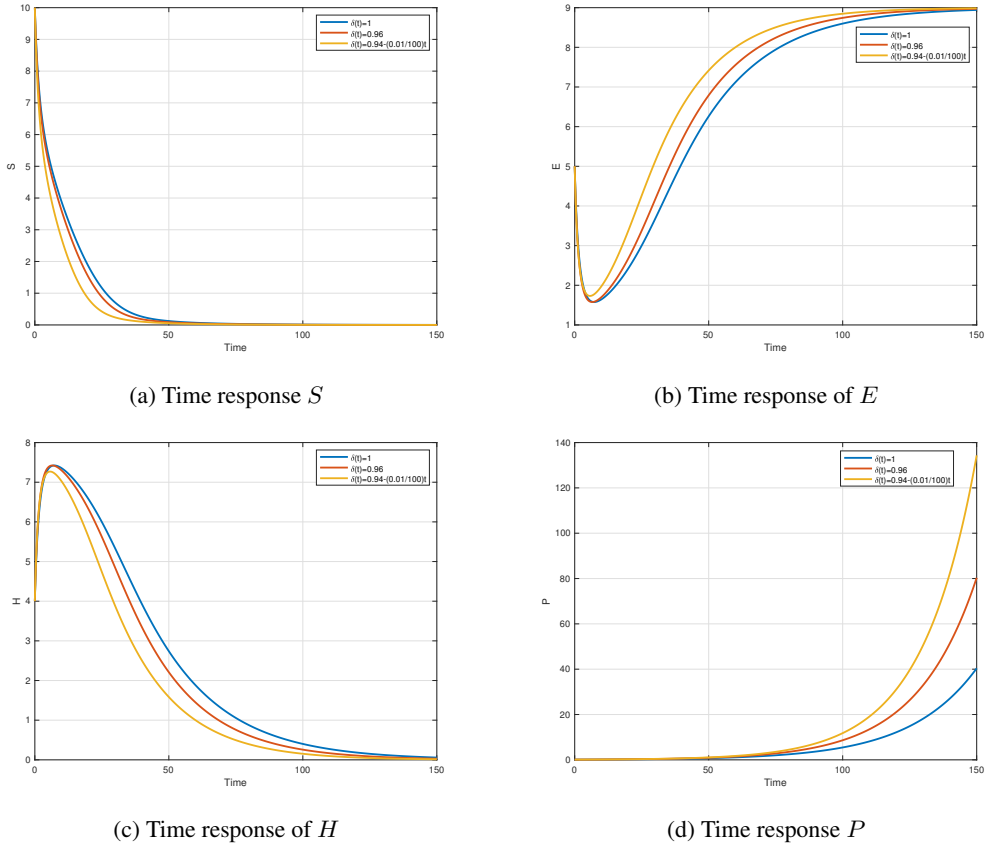


Figure 3: Comparison analysis of integer, fractional and variable order Enzyme model

6 Conclusion

In this study, we have analyzed a VOCFD model for enzyme kinetics with various orders. The existence and uniqueness solutions of the model have been established with the help of some fixed point theorems. Moreover, we implemented the VOFRK4M technique to numerically solve the model. The numerical simulations were visualized through graphical representations for different variable orders and compared with their integer and fractional-order values. The compartmental dynamics were analyzed, effectively demonstrating their growth and decay behaviors. The effectiveness and accuracy of the proposed methods are assessed through graphical analysis. The impact of variable-order values is explored, with corresponding visual representations illustrated in the figures. The findings suggest that the applied variable-order derivative operators enhance the characterization of the enzyme model dynamics. Further research can extend the model to a more realistic complex network form.

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