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Dynamics of enzyme kinetic model under the new generalized Hattaf fractional derivative

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Catalytic action is one of the most important characteristics of enzymes in chemical reactions. In this article, we propose and study a mathematical model of chemical kinetic reaction with the memory effect using the new generalized Hattaf fractional derivative. The existence and uniqueness of the solutions are established by means of fixed point theory and, finally, to support the theoretical results, we end the article with the results of numerical simulations based on a novel numerical scheme that includes the Euler method.

Keywords: *enzymatic reaction; Hattaf fractional derivative; fixed point theory; numerical simulations.*

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1. Introduction

In chemical kinetic reactions, enzymes catalyze reactions at neutral pH values and low temperatures, often at very high rates. Catalytic action is one of the crucial properties of enzymes in chemical reactions that involves lowering the reaction free energy of activation by catalyzing the transformation of substrates into products. Furthermore, enzyme mechanisms are potentially useful in various fields of physiology and biochemistry, as well as in many industrial bio-processes like textile industry and food processing.

In the literature, various models have proposed to understand and describe the dynamics of enzymatic reaction. For instance, Wong [1] studied transient-state and steady-state phases of the reaction according to the enzymatic mechanism of Michaelis and Menten [2]. In order to study the kinetic behavior at high enzyme concentrations, Cha [3] examined the Michaelis–Menten equation and three other approximations, which take into account the depletion of free substrate by binding to the enzyme. Wald et al. [4] investigated enzymatic hydrolysis of cellulose for sugar production, which offers advantages of higher conversion, low energy requirements, and mild operating conditions over other chemical conversions. Najafpour and Shan [5] focused studied on enzymatic hydrolysis of molasses by means of glucoamylase. Gan et al. [6] presented an overview, an experimental study and mathematical modelling of kinetic dynamics in heterogeneous enzymatic hydrolysis of cellulose. In 2006, Urban et al. [7] explored enzymatic microreactors in chemical analysis and kinetic studies. In [8], the authors developed a differential quasi-steady state approximate kinetic model in order to predict the behavior of complex biochemical systems. In [9], Atangana examined a model for the enzymatic control reaction using fractional derivative in Caputo sense. In 2018, Milek [10] studied hydrogen peroxide decomposition and aspergillus niger catalase deactivation at temperature varying. In [11], the authors analyzed the dynamics of two-step reversible enzymatic reaction under the Atangana–Baleanu fractional derivative [12].

In this study, we improve and generalize the model given in [11] by considering the new generalized Hattaf fractional (GHF) derivative [13] that includes the Atangana–Baleanu fractional derivative [12], the Caputo–Fabrizio fractional derivative [14] and the weighted Atangana–Baleanu fractional derivative [15].

The rest of this paper is outlined as follows. Section 2 is devoted to some preliminary results about GHF derivative. Section 3 deals with the existence and uniqueness of solutions of the proposed model. Section 4 studies the numerical simulation of the proposed model. Finally, the paper ends with a conclusion section.

2. Preliminaries

This section gives the necessary results and definitions for the elaboration of this study.

Definition 1. *Let $\alpha \in [0,1)$, $\beta, \gamma > 0$, and $f \in H^1(a,b)$. We define the GHF derivative of order α in Caputo sense of the function $f(t)$ with respect to the weight function $w(t)$ as follows [13],*

$$ {}^{C}D^{\alpha,\beta,\gamma}_{a,t,w} f(t) = \frac{N(\alpha)}{1-\alpha} \frac{1}{w(t)} \int_a^t E_\beta[-\mu_\alpha (t-\tau)^\gamma] \frac{d}{d\tau}(wf)(\tau)\, d\tau, \tag{1} $$

where $w \in C^1(a,b)$, $w, w' > 0$ on $[a,b]$, $N(\alpha)$ is a normalization function obeying $N(0) = N(1) = 1$, $\mu_\alpha = \frac{\alpha}{1-\alpha}$ and $E_\beta(t) = \sum_{k=0}^{+\infty} \frac{t^k}{\Gamma(\beta k+1)}$ is the Mittag–Leffler function of parameter β.

The GHF derivative introduced in the above definition generalizes and extends many special cases. In the fact, when $w(t) = 1$ and $\beta = \gamma = 1$, we get the Caputo–Fabrizio fractional derivative [14] given by

$$ {}^{C}D^{\alpha,1,1}_{a,t,1} f(t) = \frac{N(\alpha)}{1-\alpha} \int_a^t \exp[-\mu_\alpha (t-\tau)] f'(\tau)\, d\tau. $$

We obtain the Atangana–Baleanu fractional derivative [12] when $w(t) = 1$ and $\beta = \gamma = \alpha$, equation (1) is given by

$$ {}^{C}D^{\alpha,\alpha,\alpha}_{a,t,1} f(t) = \frac{N(\alpha)}{1-\alpha} \int_a^t E_\alpha[-\mu_\alpha (t-\tau)^\alpha] f'(\tau)\, d\tau. $$

For $\beta = \gamma = \alpha$, we get the weighted Atangana–Baleanu fractional derivative [15] given by

$$ {}^{C}D^{\alpha,\alpha,\alpha}_{a,t,w} f(t) = \frac{N(\alpha)}{1-\alpha} \frac{1}{w(t)} \int_a^t E_\alpha[-\mu_\alpha (t-\tau)^\alpha] \frac{d}{d\tau}(wf)(\tau)\, d\tau. $$

For simplicity, we denote ${}^{C}D^{\alpha,\beta,\beta}_{a,t,w}$ by $\mathcal{D}^{\alpha,\beta}_{a,w}$. By [13], the generalized fractional integral associated to $\mathcal{D}^{\alpha,\beta}_{a,w}$ is given by the following definition.

Definition 2 (Ref. [13]). *The generalized fractional integral operator associated to $\mathcal{D}^{\alpha,\beta}_{a,w}$ is defined by*

$$ \mathcal{I}^{\alpha,\beta}_{a,w} f(t) = \frac{1-\alpha}{N(\alpha)} f(t) + \frac{\alpha}{N(\alpha)} {}^{RL}\mathcal{I}^{\beta}_{a,w} f(t), \tag{2} $$

where ${}^{RL}\mathcal{I}^{\beta}_{a,w}$ is the standard weighted Riemann–Liouville fractional integral of order β defined by

$$ {}^{RL}\mathcal{I}^{\beta}_{a,w} f(t) = \frac{1}{\Gamma(\beta)} \frac{1}{w(t)} \int_a^t (t-\tau)^{\beta-1} w(\tau) f(\tau) d\tau. \tag{3} $$

Now, we recall an important theorem that we will need in the following. This theorem extends the Newton–Leibnitz formula introduced in [16, 17].

Theorem 1 (Ref. [18]). *Let $\alpha \in [0,1)$, $\beta > 0$ and $f \in H^1(a,b)$. Then we have the following property:*

$$ \mathcal{I}^{\alpha,\beta}_{a,w}\big(\mathcal{D}^{\alpha,\beta}_{a,w} f\big)(t) = f(t) - \frac{w(a) f(a)}{w(t)}. \tag{4} $$

3. The GHF enzyme kinetic model

This section constructs a mathematical chemical kinetics model involving GHF derivative. Then we divide the elements of the chemical reaction into four classes x_1, x_2, x_3 and x_4 that represent the substrate, the enzyme, the complex and the product, respectively. The dynamics of the four elements is formulated by the following nonlinear system of fractional differential equations (FDEs):

$$\begin{cases} \mathcal{D}_{a,w}^{\alpha,\beta} x_1(t) = \mu x_1 - \sigma x_1 x_2, \\ \mathcal{D}_{a,w}^{\alpha,\beta} x_2(t) = (\zeta + \mu) x_3 - \sigma x_1 x_2, \\ \mathcal{D}_{a,w}^{\alpha,\beta} x_3(t) = \sigma x_1 x_2 - (\zeta + \mu) x_3, \\ \mathcal{D}_{a,w}^{\alpha,\beta} x_4(t) = \zeta x_3, \end{cases} \tag{5}$$

subject to initial conditions $x_i(0)$ of $x_i(t)$, for $i = 1, \ldots, 4$. First, to summarize the dynamics of the system (5), the enzyme x_1 reacts with the substrate x_2 and then transforms it to product x_4. On the other hand, x_1 and x_2 combine to produce a complex x_3 at a positive rate σ. This complex x_3 then degrades to produce x_4, which releases x_2 at a positive rate ζ, and subsequently to make x_2 and x_1 at a positive rate μ.

3.1. Existence and uniqueness of solutions

In this subsection, let $\mathcal{E} = [0, t_{\max}]$ and $\mathcal{B} = C(\mathcal{E}, \mathbb{R})$ be the Banach space of continuous functions from $\mathcal{E}$ to $\mathbb{R}$ defined with the norm

$$\|x_i\| = \sup\{|x_i(t)| \colon t \in \mathcal{E}\} \text{ for } i = 1, \ldots, 4.$$

By using Theorem 1, the fractional chemical kinetics model described in (5) can be written in the following form

$$\begin{aligned} x_1(t) &= x_{1,0}(t) + \frac{1-\alpha}{N(\alpha)} G_1(t, x_1(t)) + \frac{\alpha}{N(\alpha)\Gamma(\beta) w(t)} \int_0^t (t-s)^{\beta-1} w(s) G_1(s, x_1(s))\, ds, \\ x_2(t) &= x_{2,0}(t) + \frac{1-\alpha}{N(\alpha)} G_2(t, x_2(t)) + \frac{\alpha}{N(\alpha)\Gamma(\beta) w(t)} \int_0^t (t-s)^{\beta-1} w(s) G_2(s, x_2(s))\, ds, \\ x_3(t) &= x_{3,0}(t) + \frac{1-\alpha}{N(\alpha)} G_3(t, x_3(t)) + \frac{\alpha}{N(\alpha)\Gamma(\beta) w(t)} \int_0^t (t-s)^{\beta-1} w(s) G_3(s, x_3(s))\, ds, \\ x_4(t) &= x_{4,0}(t) + \frac{1-\alpha}{N(\alpha)} G_4(t, x_4(t)) + \frac{\alpha}{N(\alpha)\Gamma(\beta) w(t)} \int_0^t (t-s)^{\beta-1} w(s) G_4(s, x_4(s))\, ds, \end{aligned} \tag{6}$$

where $x_{i,0}(t) = \frac{x_i(0) w(0)}{w(t)}$ for $i = 0, \ldots, 4$ and

$$\begin{cases} G_1(t, x_1(t)) = \mu x_1 - \sigma x_1 x_2, \\ G_2(t, x_2(t)) = (\zeta + \mu) x_3 - \sigma x_1 x_2, \\ G_3(t, x_3(t)) = \sigma x_1 x_2 - (\zeta + \mu) x_3, \\ G_4(t, x_4(t)) = \zeta x_3. \end{cases} \tag{7}$$

We can verify that the functions G_1, G_2, G_3 and G_4 satisfy the Lipschitz conditions with L_i Lipschitz constant satisfying $L_i < 1$, for $i = 0, \ldots, 4$.

By the following recursive formula,

$$\begin{aligned}
x_{1,n}(t) &= x_{1,0}(t) + \frac{1-\alpha}{N(\alpha)} G_1\left(t, x_{1,n-1}(t)\right) + \frac{\alpha}{N(\alpha)\Gamma(\beta)w(t)} \int_0^t (t-s)^{\beta-1} w(s) G_1\left(s, x_{1,n-1}(s)\right) ds,\\
x_{2,n}(t) &= x_{2,0}(t) + \frac{1-\alpha}{N(\alpha)} G_2\left(t, x_{2,n-1}(t)\right) + \frac{\alpha}{N(\alpha)\Gamma(\beta)w(t)} \int_0^t (t-s)^{\beta-1} w(s) G_2\left(s, x_{2,n-1}(s)\right) ds,\\
x_{3,n}(t) &= x_{3,0}(t) + \frac{1-\alpha}{N(\alpha)} G_3\left(t, x_{3,n-1}(t)\right) + \frac{\alpha}{N(\alpha)\Gamma(\beta)w(t)} \int_0^t (t-s)^{\beta-1} w(s) G_3\left(s, x_{3,n-1}(s)\right) ds,\\
x_{4,n}(t) &= x_{4,0}(t) + \frac{1-\alpha}{N(\alpha)} G_4\left(t, x_{4,n-1}(t)\right) + \frac{\alpha}{N(\alpha)\Gamma(\beta)w(t)} \int_0^t (t-s)^{\beta-1} w(s) G_4\left(s, x_{4,n-1}(s)\right) ds,
\end{aligned} \tag{8}$$

we write the difference between the successive terms as

$$\begin{aligned}
A_n(t) &= x_{1,n}(t) - x_{1,n-1}(t)\\
&= \frac{1-\alpha}{N(\alpha)} \left[G_1\left(t, x_{1,n-1}(t)\right) - G_1\left(t, x_{1,n-2}(t)\right)\right]\\
&\quad + \frac{\alpha}{N(\alpha)\Gamma(\beta)w(t)} \int_0^t (t-s)^{\beta-1} w(s) \left[G_1\left(s, x_{1,n-1}(s)\right) - G_1\left(s, x_{1,n-2}(s)\right)\right] ds,\\
B_n(t) &= x_{2,n}(t) - x_{2,n-1}(t)\\
&= \frac{1-\alpha}{N(\alpha)} \left[G_1\left(t, x_{2,n-1}(t)\right) - G_1\left(t, x_{2,n-2}(t)\right)\right]\\
&\quad + \frac{\alpha}{N(\alpha)\Gamma(\beta)w(t)} \int_0^t (t-s)^{\beta-1} w(s) \left[G_2\left(s, x_{2,n-1}(s)\right) - G_2\left(s, x_{2,n-2}(s)\right)\right] ds,\\
C_n(t) &= x_{3,n}(t) - x_{3,n-1}(t)\\
&= \frac{1-\alpha}{N(\alpha)} \left[G_3\left(t, x_{3,n-1}(t)\right) - G_3\left(t, x_{3,n-2}(t)\right)\right]\\
&\quad + \frac{\alpha}{N(\alpha)\Gamma(\beta)w(t)} \int_0^t (t-s)^{\beta-1} w(s) \left[G_3\left(s, x_{3,n-1}(s)\right) - G_3\left(s, x_{3,n-2}(s)\right)\right] ds,\\
D_n(t) &= x_{4,n}(t) - x_{4,n-1}(t)\\
&= \frac{1-\alpha}{N(\alpha)} \left[G_4\left(t, x_{4,n-1}(t)\right) - G_4\left(t, x_{4,n-2}(t)\right)\right]\\
&\quad + \frac{\alpha}{N(\alpha)\Gamma(\beta)w(t)} \int_0^t (t-s)^{\beta-1} w(s) \left[G_4\left(s, x_{4,n-1}(s)\right) - G_4\left(s, x_{4,n-2}(s)\right)\right] ds.
\end{aligned}$$

We verify immediately that

$$\begin{aligned}
x_{1,n}(t) - x_{1,0}(t) &= \sum_{i=1}^{n} A_i(t),\\
x_{2,n}(t) - x_{2,0}(t) &= \sum_{i=1}^{n} B_i(t),\\
x_{3,n}(t) - x_{3,0}(t) &= \sum_{i=1}^{n} C_i(t),\\
x_{4,n}(t) - x_{4,0}(t) &= \sum_{i=1}^{n} D_i(t).
\end{aligned} \tag{9}$$

By the above result, we write the following theorem of existence and uniqueness of solutions of model (5).

Theorem 2. *The GHF fractional chemical kinetics model (5) has a unique solution for* $t \in [0, t_{\max}]$ *if* $\left(\frac{1-\alpha}{N(\alpha)} + \frac{\alpha t_{\max}^{\beta}}{N(\alpha)\Gamma(\beta+1)}\right) L_i < 1$, *for* $i = 1, \ldots, 4$.

Proof. Since the functions G_i satisfy the Lipschitz conditions, we can prove

$$\begin{aligned}
\|A_n(t)\| &\leqslant \|x_{1,0}\| \left[\frac{1-\alpha}{N(\alpha)}L_1 + \frac{\alpha t_{max}^{\beta}}{N(\alpha)\Gamma(\beta+1)}L_1\right]^n,\\
\|B_n(t)\| &\leqslant \|x_{2,0}\| \left[\frac{1-\alpha}{N(\alpha)}L_2 + \frac{\alpha t_{max}^{\beta}}{N(\alpha)\Gamma(\beta+1)}L_2\right]^n,\\
\|C_n(t)\| &\leqslant \|x_{3,0}\| \left[\frac{1-\alpha}{N(\alpha)}L_3 + \frac{\alpha t_{max}^{\beta}}{N(\alpha)\Gamma(\beta+1)}L_3\right]^n,\\
\|D_n(t)\| &\leqslant \|x_{4,0}\| \left[\frac{1-\alpha}{N(\alpha)}L_4 + \frac{\alpha t_{max}^{\beta}}{N(\alpha)\Gamma(\beta+1)}L_4\right]^n.
\end{aligned} \tag{10}$$

Therefore, the above-mentioned sequences exist and satisfy $\|A_n(t)\| \to 0$, $\|B_n(t)\| \to 0$, $\|C_n(t)\| \to 0$, $\|D_n(t)\| \to 0$ as $n \to +\infty$. On the other hand, by applying the triangular inequality, we get

$$\begin{aligned}
\|x_{1,n+j} - x_{1,n}\| &\leqslant \|x_{1,0}\| \sum_{k=n+1}^{n+j} \left[\frac{1-\alpha}{N(\alpha)}L_1 + \frac{\alpha t_{\max}^{\beta}}{N(\alpha)\Gamma(\beta+1)}L_1\right]^k,\\
\|x_{2,n+j} - x_{2,n}\| &\leqslant \|x_{2,0}\| \sum_{k=n+1}^{n+j} \left[\frac{1-\alpha}{N(\alpha)}L_2 + \frac{\alpha t_{\max}^{\beta}}{N(\alpha)\Gamma(\beta+1)}L_2\right]^k,\\
\|x_{3,n+j} - x_{3,n}\| &\leqslant \|x_{3,0}\| \sum_{k=n+1}^{n+j} \left[\frac{1-\alpha}{N(\alpha)}L_3 + \frac{\alpha t_{\max}^{\beta}}{N(\alpha)\Gamma(\beta+1)}L_3\right]^k,\\
\|x_{4,n+j} - x_{4,n}\| &\leqslant \|x_{4,0}\| \sum_{k=n+1}^{n+j} \left[\frac{1-\alpha}{N(\alpha)}L_4 + \frac{\alpha t_{\max}^{\beta}}{N(\alpha)\Gamma(\beta+1)}L_4\right]^k.
\end{aligned} \tag{11}$$

Since $\left(\frac{1-\alpha}{N(\alpha)} + \frac{\alpha t_{\max}^{\beta}}{N(\alpha)\Gamma(\beta+1)}\right) L_i < 1$, we deduce that $x_{i,n}$ are Cauchy sequences. Thus, for all $i = 0, \ldots, 4$, $x_{i,n}$ are uniformly convergent. Applying this result to system (8), we conclude that model (5) has a unique solution. ∎

4. Numerical simulations

In this section, we apply the numerical scheme cited in [19] to formulate the equations of the GHF chemical kinetic model (5) in the following approximations

$$\begin{aligned}
x_1(t_{n+1}) &= \frac{x_1(0)w(0)}{w(t_n)} + \frac{1-\alpha}{N(\alpha)}G_1((t, x_1(t_n)) + \frac{\alpha}{N(\alpha)\Gamma(\beta+1)}\frac{h^{\beta}}{w(t_n)}\sum_{k=0}^{n} w(t_k)G_1((t_k, x_1(t_k))\mathcal{A}_{n,k}^{\beta},\\
x_2(t_{n+1}) &= \frac{x_2(0)w(0)}{w(t_n)} + \frac{1-\alpha}{N(\alpha)}G_2((t, x_2(t_n)) + \frac{\alpha}{N(\alpha)\Gamma(\beta+1)}\frac{h^{\beta}}{w(t_n)}\sum_{k=0}^{n} w(t_k)G_2((t_k, x_2(t_k))\mathcal{A}_{n,k}^{\beta},\\
x_3(t_{n+1}) &= \frac{x_3(0)w(0)}{w(t_n)} + \frac{1-\alpha}{N(\alpha)}G_3((t, x_3(t_n)) + \frac{\alpha}{N(\alpha)\Gamma(\beta+1)}\frac{h^{\beta}}{w(t_n)}\sum_{k=0}^{n} w(t_k)G_3((t_k, x_3(t_k))\mathcal{A}_{n,k}^{\beta},\\
x_4(t_{n+1}) &= \frac{x_4(0)w(0)}{w(t_n)} + \frac{1-\alpha}{N(\alpha)}G_4(t, x_4(t_n)) + \frac{\alpha}{N(\alpha)\Gamma(\beta+1)}\frac{h^{\beta}}{w(t_n)}\sum_{k=0}^{n} w(t_k)G_4((t_k, x_4(t_k))\mathcal{A}_{n,k}^{\beta},
\end{aligned}$$

where

$$\mathcal{A}_{n,k}^{\beta} = (n-k+1)^{\beta} - (n-k)^{\beta}.$$

To support the theoretical results, we give the following graphs for different values of the parameter α in order to study the impact of the memory effect on the system with the following initial conditions

$x_1(0) = 0.17$, $x_2(0) = 0.1000005$, $x_3(0) = 0.01005$ and $x_4(0) = 0$. Also, we choose $\mu = 0.48$, $\sigma = 0.48$, $\zeta = 0.48$, $\beta = 0.9$ and $w(t) = 1$.

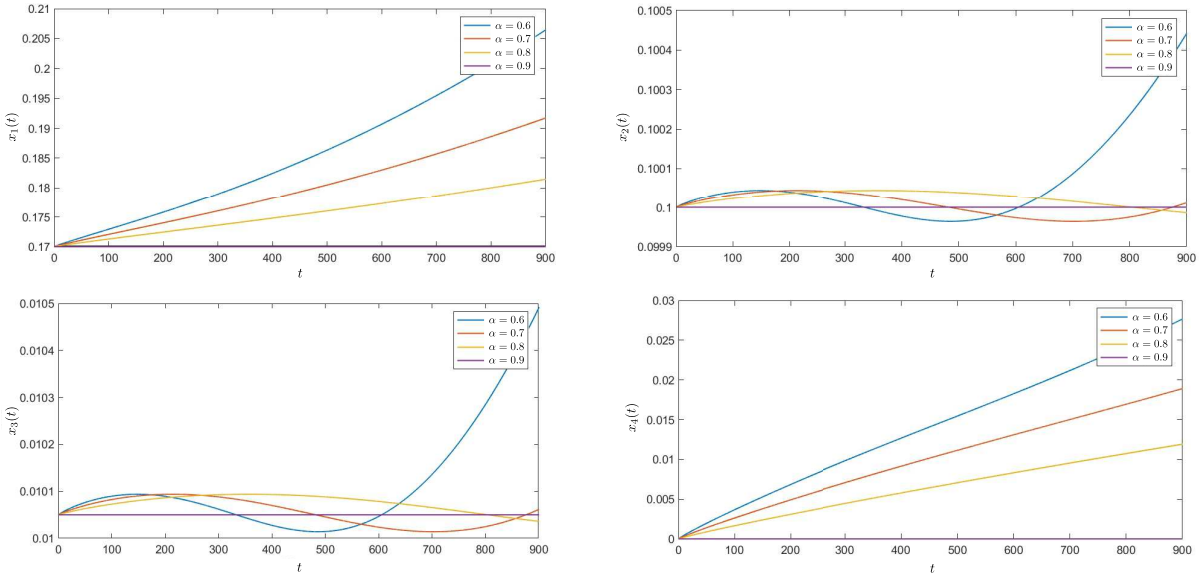

Fig. 1. The impact of the memory effect on the dynamics of system (5).

Figure 1 shows the numerical solutions of system (5) including substrate, enzyme, complex and product for different values of fractional order α. Based on such figure, we conclude that the memory has a significant effect on the dynamics of model (5). Therefore, it is more interesting to study the dynamics of enzymatic reaction by taking into account the effect of memory.

5. Conclusion

In this article, we have explored the role of catalytic action in enzymatic chemical reactions. Our study focused on developing and examining a mathematical model for chemical kinetic reactions that incorporates memory effects using the generalized Hattaf fractional derivative. Additionally, by applying fixed point theory, we have demonstrated the existence and uniqueness of solutions. To support our findings, we performed numerical simulations using a numerical scheme that covers the Euler method. This comprehensive study contributes to the expanding body of knowledge in enzyme catalysis and paves the way for further advancements in understanding and manipulating chemical reactions with memory effects.

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Динаміка ферментативної кінетичної моделі за новою узагальненою дробовою похідною Хаттафа

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Каталітична дія є однією з найважливіших характеристик ферментів у хімічних реакціях. У цій статті пропонується та досліджується математична модель хімічної кінетичної реакції з ефектом пам'яті з використанням нової узагальненої дробової похідної Хаттафа. Існування та єдиність розв'язків встановлено за допомогою теорії нерухомої точки, і, нарешті, щоб підтвердити теоретичні результати, закінчуємо чисельним моделюванням на основі нової чисельної схеми, яка включає метод Ейлера.

Ключові слова: *ферментативна реакція; дробова похідна Хаттафа; теорія нерухомої точки; чисельне моделювання.*