Approximate solutions of the biochemical reaction kinetics model for methane production from anaerobic digestion process of cellulose using sigmoid-weighted neural networks

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Research Article

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Abstract Anaerobic digestion process is a spreading rapidly biotechnology for conversion of various organic wastes into bioenergy. This process can be modelled as a biochemical reaction kinetics. This approach is useful for analysis of the process. For this reason, efficient numerical methods are needed to solve this type of model. The main contribution of this study is to solve the biochemical reaction kinetics model for methane production from anaerobic digestion process of cellulose. This model provides a system of ordinary differential equations. For solving this system, a method is designed based on the universal approximation capability of a three layer feedforward sigmoid-weighted neural networks with Adam optimization algorithm. This method is illustrated with numerical simulations. Moreover, the classical numerical methods such as Runge-Kutta method (RK45) and sigmoid neural networks are presented to show that all methods yield similar results.

Keywords Anaerobic digestion process · Biochemical reaction kinetics · Universal approximation · Sigmoid-weighted neural networks · Adam optimization algorithm.

Mathematics Subject Classification (2020) MSC 41A81 · 68T07 · 34-11

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1 Introduction

Anaerobic digestion process is a sustainable biotechnology to obtain bioenergy. This process comprises sequences of biochemical reactions to convert biomass resources into biogas in the absence of oxygen. Biogas is a colorless and blue burning gas such as methane and dioxide carbon. Anaerobic digestion process has been utilized for many years. This process has been received much attention due to the increasing of energy prices in the 1970s [1]. The interest in this biotechnology still continues due to environment benefits [2]. European countries have agreed to change their gas gird to biogas by 2050 [3]. Anaerobic digestion process is a complex biological process because of the inclusion of diverse microbial species in a blended populations. Anaerobic digestion process can be represented into four complex stages involving hydrolysis, acidogenesis, acetogenesis, and methanogenesis [4]. Cellulose can be used as substrate for methane production in anaerobic digestion process. Methane produces few air pollutions compare to other fules [5]. In the hydrolysis stage, cellulose is broken down into glucose. In the next stage, the glucose is converted to butyric acid, carbon dioxide and hydrogen. In the third stage, butyric acid, carbon dioxide and hydrogen are converted to acetic acid and methane. The last stage is divided into two main groups i.e. acetoclastic methanogenesis and hydogenotrophic. In the first group, methane is produced from acetic acid by methanogen microorganism. In the second group, methane is produced from hydrogen and carbon dioxide by methanogen microorganism.

On the other hand, the anaerobic digestion process requires the development of appropriate biochemical reaction kinetics models which adequately show the key process that happens. This requires of development of models is determined by the fact that there is no universal model for predicting the anaerobic digestion process of different substrates. Due to improvement in computational techniques, several researches have been done for modelling the anaerobic digestion process in different practical point of views [6–9]. To the best of our knowledge, there are few works dealing with approximations solutions of the biochemical reaction kinetics model of an anaerobic digestion process such as Runge-Kutta method [10], modified Adomian decomposition method [11], Rosenbrock method [12]. The system of ordinary differential equations has been traditionally described the biochemical reaction kinetics [13].

The main objective of this study is to make an efficient approximation solutions of Silva and Bertoli 's biochemical reaction kinetics model for methane production from anaerobic digestion process of cellulose [14]. The model provides a system of ordinary differential equations associated to the previously described stages. The system of ordinary differential equations is first order nonlinear. Recently, we have proposed a three layer feedforward sigmoid-weighted neural networks for approximation problems [15,16]. In this study, we propose our method to approximate the solutions of this system of ordinary differential equations. This method is based on the universal approximation capability of a three layer feedforward sigmoid-weighted neural networks Adam optimization algorithm. We show that the proposed method and the numerical

Table 1 The description of the variables in the biochemical reaction kinetics model

Variable	Chemical formula	Chemical compound
y_1	$C_6H_{10}O_5$	Cellulose
y_2	$C_6H_{12}O_6$	Glucose
y_3	$C_4H_8O_2$	Butyric acid
y_4	$C_2H_4O_2$	Acetic acid
y_5	CH_4	Methane
y_6	CO_2	Carbon dioxide
y_7	H_2	Hydrogen
y_8	H_2O	Water

Table 2 The biochemical reactions for methane production from anaerobic digestion process of cellulose

Reaction	Rate
$C_6H_{10}O_5 + H_2O = C_6H_{12}O_6$	$k_0[C_6H_{10}O_5][H_2O]$
$C_6H_{12}O_6 = C_4H_8O_2 + 2CO_2 + 2H_2O$	$k_1[C_6H_{12}O_6]$
$C_4H_8O_2 + H_2O + \frac{1}{2}CO_2 = 2C_2H_4O_2 + \frac{1}{2}CH_4$	$k_2[C_4H_8O_2][H_2O][CO_2]^{1/2}$
$\frac{1}{2}CO_2 + 2H_2 = \frac{1}{2}CH_4 + H_2O$	$k_3[CO_2]^{1/2}[H_2]^2$
$2C_2H_4O_2 = 2CH_4 + 2CO_2$	$k_4[C_2H_4O_2]^2$

methods such as RK45 and sigmoid neural networks yield similar results.

This study is structured as follows. In Section 2, the biochemical reaction kinetics model for an anaerobic digestion process is presented. In Section 3, the neural network approximation method for solving this model is described. In Section 4, the results of simulations are provided. Finally, in Section 5, conclusions and new directions for future works are given.

2 The biochemical reaction kinetics model for methane production from anaerobic digestion process of cellulose

The biochemical reaction kinetics model is capable of representing the qualitative behavior of an anaerobic digestion process. In the anaerobic digestion process, cellulose is used as a substrate for the production of methane. The chemical compounds included within the anaerobic digestion process which are

Table 3 The values of the parameters in the biochemical reaction kinetics model

Parameter	Value
k_0	1.0000
k_1	1.1125
k_2	1.014
k_3	1.054
k_4	1.015

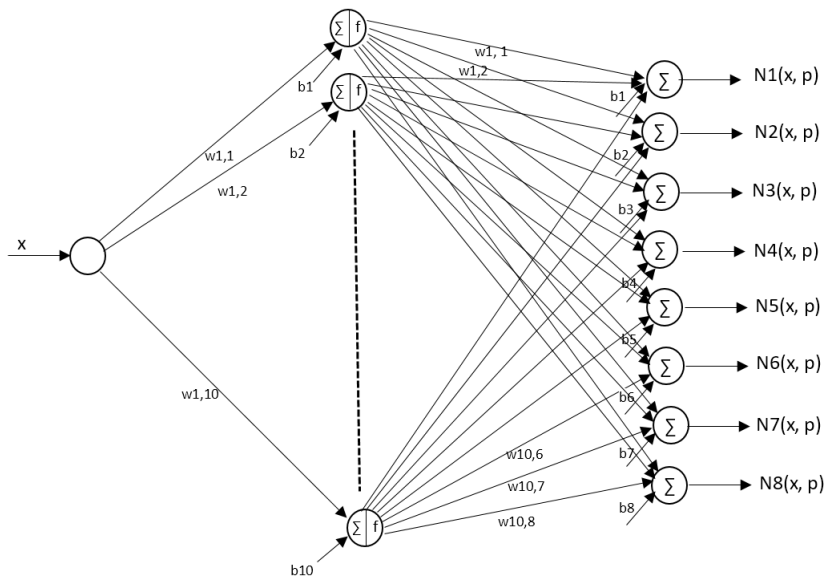

Fig. 1 The architecture of the proposed neural networks

related with their chemical formulas and abbreviations are presented in Table 1. The set of the biochemical reactions for the anaerobic digestion process are given in Table 2. The following model is composed of five reactions and eight species. This model is governed by a system of ordinary differential equations with few variables as follows.

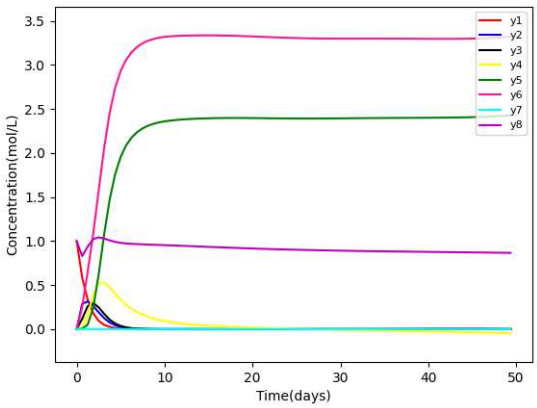

Fig. 2 The approximate solutions for model using the proposed method

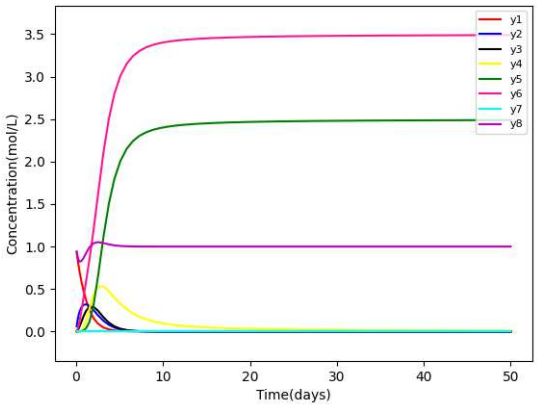

Fig. 3 The approximate solutions for model using RK45

$$
\begin{cases}
\dfrac{dy_1(t)}{dt} = k_0 y_1(t) y_8(t), \\[2ex]
\dfrac{dy_2(t)}{dt} = k_0 y_1(t) y_8(t) - k_1 y_2(t), \\[2ex]
\dfrac{dy_3(t)}{dt} = k_1 y_2(t) - k_2 y_3(t) y_8(t) y_6(t)^{\frac{1}{2}}, \\[2ex]
\dfrac{dy_4(t)}{dt} = 2k_2 y_3(t) y_8(t) y_6(t)^{\frac{1}{2}} - 2k_4 y_4(t)^2, \\[2ex]
\dfrac{dy_5(t)}{dt} = \frac{1}{2} k_2 y_3(t) y_8(t) y_6(t)^{\frac{1}{2}} + \frac{1}{2} k_3 y_6(t)^{\frac{1}{2}} y_7(t)^2 + 2k_4 y_4(t)^2, \\[2ex]
\dfrac{dy_6(t)}{dt} = 2k_1 y_2(t) - \frac{1}{2} y_2 y_3(t) y_8(t) y_6(t)^{\frac{1}{2}} - \frac{1}{2} k_3 y_6(t)^{\frac{1}{2}} y_7(t)^2 + 2k_4 y_4(t)^2, \\[2ex]
\dfrac{dy_7(t)}{dt} = 2k_1 y_2(t) - 2k_3 y_6^{\frac{1}{2}} y_7(t)^2, \\[2ex]
\dfrac{dy_8(t)}{dt} = -k_0 y_1(t) y_8(t) - k_2 y_2(t) y_8(t) y_6(t)^{\frac{1}{2}} + k_3 y_6(t)^{\frac{1}{2}} y_7(t)^2,
\end{cases}
\tag{1}
$$

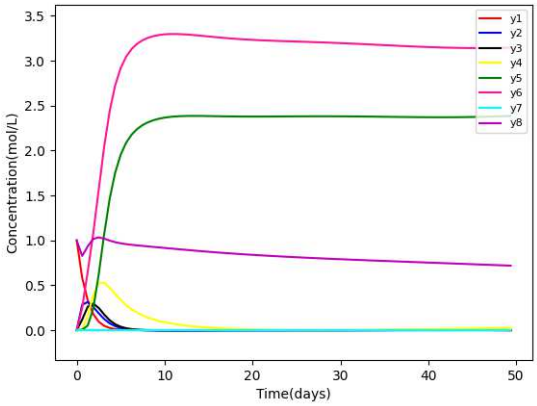

Fig. 4 The approximate solutions for model using sigmoid neural networks

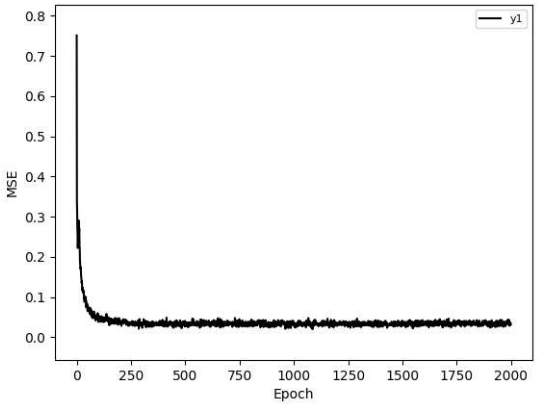

Fig. 5 The convergence of y_1

with initial values

$y_1(0) = 1$, $y_2(0) = 0$, $y_3(0) = 0$, $y_4(0) = 0$, $y_5(0) = 0$, $y_6(0) = 0$, $y_7(0) = 0$ and $y_8(0) = 1$.

The parameter values of the model are shown in Table 3.

In the next section, we will present our approach and discuss concerning the neural networks approximation method for solving this system of ordinary differential equations.

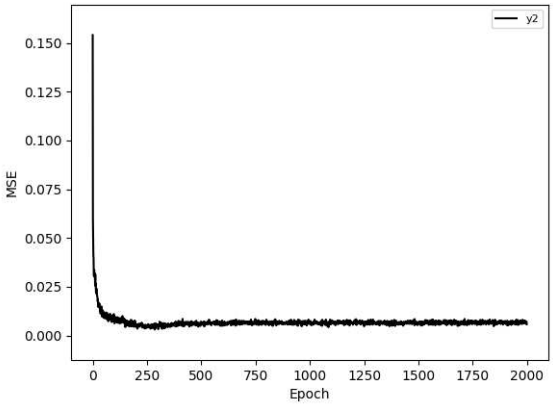

Fig. 6 The convergence of y_2

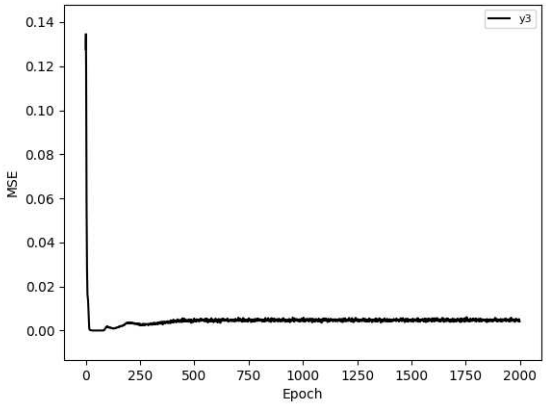

Fig. 7 The convergence of y_3

3 The sigmoid-weighted neural networks for solving the biochemical reaction kinetics model

The universal approximation capability of feedforward neural networks in the weighted space of continuous functions i.e. any weighted smooth function can be approximated by a three layer feedforward artificial neural networks arbitrarily well [17]. Elfwing et al. [18] introduced sigmoid-weighted neural networks and showed that this type of neural networks are more accurate than the traditional sigmoid neural networks. We use the three layer feedforward sigmoid-weighted neural networks with Adam optimization algorithm to find the approximate solutions of system of ordinary differential equations with eight variables. The universal approximation capability of a three layer feed-

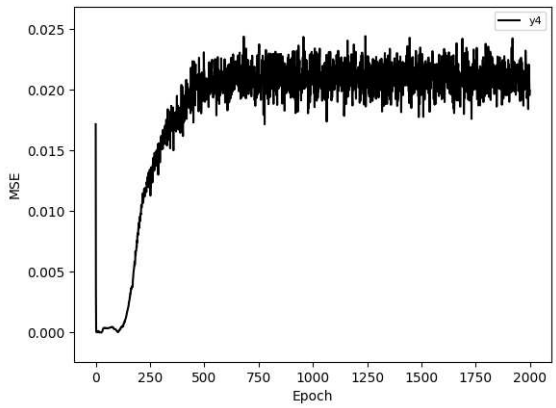

Fig. 8 The convergence of y_4

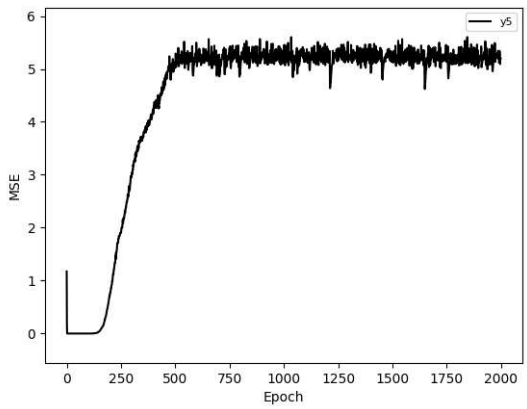

Fig. 9 The convergence of y_5

forward sigmoid-weighted neural networks appears to be an essential key point to solve the system of ordinary differential equations. The activation function of sigmoid-weighted neural networks is introduced as follows:

$$a(x) = \sigma(x)(1 + x(1 - \sigma(x))). \tag{2}$$

We have:

$$\begin{cases} \dfrac{dy_r}{dx} = f_r(x, y_1, ..., y_n) \quad r = 1, 2, ..., 8 \quad \text{and} \quad x \in [a, b], \\ \\ y_r(a) = A_r, \quad r = 1, 2, ..., 8. \end{cases} \tag{3}$$

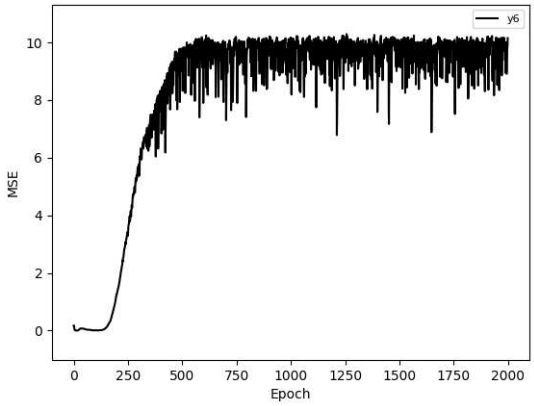

Fig. 10 The convergence of y_6

The trial solution is as follows:

$$y_{t_r}(x, p_r) = A_r + (x - a)N_r(x, p_r) \qquad r = 1, 2, ..., 8 \tag{4}$$

For each $r, N_r(x, p_r)$ is the output of the three layer feedforward sigmoid-weighted neural networks. From Eq. (4), we get

$$\frac{dy_{t_r}(x, p_r)}{dx} = N_r(x, p_r) + (x - a)\frac{dN_r(x, p_r)}{dx} \qquad r = 1, 2, ..., 8 \tag{5}$$

We define the error function as:

$$E(x, p) = \sum_{i=1}^{h}\sum_{r=1}^{8}\frac{1}{2}\left(\frac{dy_{t_r}(x_i, p_r)}{dx} - f_r\big(x_i, y_{t_1}(x_i, p_1), y_{t_2}(x_i, p_2), ..., y_{t_8}(x_i, p_8)\big)\right)^2. \tag{6}$$

The architecture of the proposed neural networks is shown in Fig. 1. The learning rate is 0.001 and the number of epoches is 2000.

4 Numerical Results

In this section, in Table 4, we show the numerical approximation solutions of the proposed method. We show the approximation solutions of the model using the proposed method, RK45, sigmoid neural networks in Figs. 2, 3, 4. We also show the convergence of approximate solutions of the model using the proposed method in Figs. 5, 6, 7, 8, 9, 10, 11, 12.

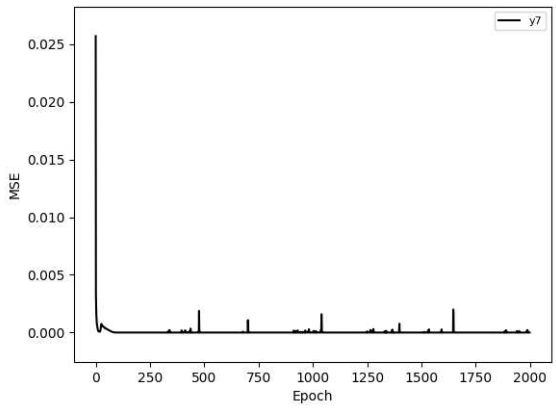

Fig. 11 The convergence of y_7

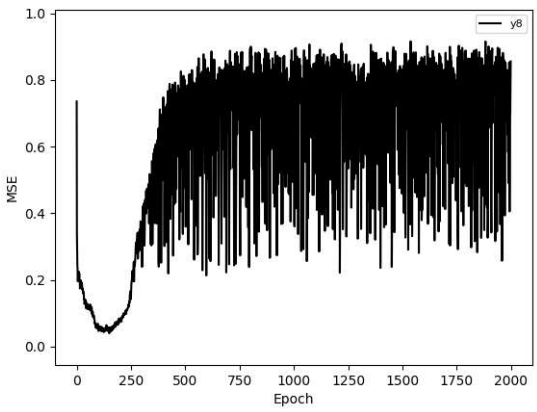

Fig. 12 The convergence of y_8

5 Conclusions

Certain microorganisms in the anaerobic digestion process produces biogas through sequeneces of four stages known as hydrolysis, acidogenesis, acetogenesis, and methanogenesis. In this anaerobic digestion process, cellulose was used as a substrate for the production of methane. This process has been formulated by the system of ordinary differential equations. We have obtained the approximation solutions of this system using the sigmoid-weighted neural networks approximation method. Our method and the classical methods show the similar results. For future works, our method can be extended to various kinds of anaerobic digestion process such as industrial waste water, sewage sludge, manure, and organic fraction of municipal wastes. Moreover, this study pro-

Table 4 Approximate solutions for model using the proposed method

x	y1	y2	y3	y4	y5	y6	y7	y8
0.0000	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000
1.2500	0.3360	0.3142	0.2599	0.1602	0.0507	0.6529	0.0000	0.9375
2.5000	0.0942	0.1904	0.2477	0.5231	0.6224	1.5715	0.0000	1.0421
3.7500	0.0250	0.0756	0.1083	0.4745	1.4714	2.4559	0.0000	1.0079
5.0000	0.0066	0.0251	0.0366	0.3336	1.9562	2.9322	0.0000	0.9800
6.2500	0.0019	0.0072	0.0111	0.2287	2.1766	3.1463	0.0000	0.9686
7.5000	-0.0001	0.0011	0.0028	0.1621	2.2806	3.2470	0.0000	0.9629
8.7500	-0.0012	-0.0008	0.0004	0.1201	2.3328	3.2961	0.0000	0.9583
10.0000	-0.0010	-0.0014	-0.0003	0.0923	2.3600	3.3194	0.0000	0.9538
11.2500	-0.0002	-0.0018	-0.0005	0.0726	2.3752	3.3297	0.0000	0.9491
12.5000	0.0006	-0.0021	-0.0007	0.0580	2.3845	3.3342	0.0000	0.9442
13.7500	0.0007	-0.0022	-0.0008	0.0471	2.3907	3.3361	0.0000	0.9393
15.0000	0.0003	-0.0023	-0.0007	0.0387	2.3950	3.3365	0.0000	0.9344
16.2500	-0.0003	-0.0022	-0.0007	0.0321	2.3975	3.3355	0.0000	0.9295
17.5000	-0.0009	-0.0021	-0.0006	0.0267	2.3986	3.3330	0.0000	0.9247
18.7500	-0.0011	-0.0020	-0.0005	0.0222	2.3985	3.3293	0.0000	0.9202
20.0000	-0.0010	-0.0019	-0.0005	0.0181	2.3975	3.3246	0.0000	0.9159
21.2500	-0.0006	-0.0019	-0.0005	0.0143	2.3961	3.3194	0.0000	0.9119
22.5000	-0.0001	-0.0019	-0.0006	0.0107	2.3947	3.3143	0.0000	0.9082
23.7500	0.0004	-0.0019	-0.0006	0.0074	2.3934	3.3097	0.0000	0.9048
25.0000	0.0009	-0.0020	-0.0007	0.0042	2.3927	3.3060	0.0000	0.9016
26.2500	0.0012	-0.0019	-0.0007	0.0012	2.3924	3.3032	0.0000	0.8987
27.5000	0.0013	-0.0019	-0.0007	-0.0016	2.3927	3.3014	0.0000	0.8960
28.7500	0.0012	-0.0018	-0.0006	-0.0043	2.3934	3.3004	0.0000	0.8936
30.0000	0.0010	-0.0017	-0.0005	-0.0068	2.3944	3.3000	0.0000	0.8913
31.2500	0.0007	-0.0015	-0.0003	-0.0093	2.3955	3.2999	0.0000	0.8891
32.5000	0.0005	-0.0013	-0.0002	-0.0117	2.3966	3.3000	0.0000	0.8872
33.7500	0.0003	-0.0011	0.0000	-0.0140	2.3976	3.3001	0.0000	0.8853
35.0000	0.0003	-0.0009	0.0002	-0.0163	2.3985	3.2999	0.0000	0.8836
36.2500	0.0004	-0.0007	0.0003	-0.0187	2.3992	3.2996	0.0000	0.8819
37.5000	0.0007	-0.0006	0.0005	-0.0211	2.3998	3.2990	0.0000	0.8803
38.7500	0.0012	-0.0004	0.0006	-0.0235	2.4003	3.2982	0.0000	0.8788
40.0000	0.0017	-0.0004	0.0007	-0.0260	2.4009	3.2975	0.0000	0.8773
41.2500	0.0023	-0.0003	0.0007	-0.0286	2.4018	3.2971	0.0000	0.8759
42.5000	0.0028	-0.0003	0.0007	-0.0312	2.4030	3.2971	0.0000	0.8745
43.7500	0.0031	-0.0004	0.0007	-0.0340	2.4050	3.2980	0.0000	0.8730
45.0000	0.0032	-0.0005	0.0007	-0.0367	2.4078	3.3000	0.0000	0.8716
46.2500	0.0029	-0.0006	0.0006	-0.0395	2.4117	3.3035	0.0000	0.8701
47.5000	0.0020	-0.0008	0.0005	-0.0423	2.4171	3.3089	0.0000	0.8686
48.7500	0.0005	-0.0009	0.0004	-0.0451	2.4241	3.3166	0.0000	0.8671

vides a basis for designing biochemical reaction kinetics fractional models of anaerobic digestion process as the next generation of mathematical models.

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Compliance with ethical standards

Conflict of interest All authors declare that they have no conflict of interest.

Research involving human participants and/or animals This article does not contain any studies with human participants or animals performed by any of the authors.

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