Revista Eletrônica
Paulista de Matemática

ISSN 2316-9664
v. 22, n. 2, set. 2022
Edição Brazilian Symposium on
Fractional Calculus

Fractional model applied to fermentation process kinetics

Hugo Pinheiro
Aerospace Engineering
State University of Maranhao
hugopinheiro@aluno.uema.br

Felix Silva Costa
Aerospace Engineering
State University of Maranhao
felix@cecen.uema.br

Abstract

Biofuels are promising alternatives to partially or fully replace oil and natural gas-based fuels in combustion engines due to less environmental impact than fossil fuels. The production of biofuels through alcoholic fermentation in chemical reactors has been an increasing interest to the industry. Several kinetic models have been examined to determine the kinetics of fermentation of microorganisms. The study and determination of this kinetic model are considered the most important step of a fermentative process since it will define the rate of production and consumption of the main constituents. The mathematical method used to model the chemical reactor equation is based on fractional calculations, more specifically the Caputo fractional derivative is applied in the Monod equation, which is responsible for modeling the reactors. It is noteworthy that fractional derivatives are an excellent tool for describing processes involving the so-called memory effect and heredity properties since in many cases they refine the solution.
Keywords: Cellular growth. fractional derivative. kinetic model. Monod equation. Saccharomyces cerevisiae.

1 Introduction

The use of fossil fuels for power generation has become a subject widely discussed today. The intense use of high carbon systems leads to dependence on fossil fuels, which becomes an obstacle in the transition to low carbon systems (SATO; ELLIOT; SCHUMER, 2021). However, due to increasing climate change and environmental impacts, the search for alternative fuels to meet global energy demand has been growing exponentially, contributing to the reduction of greenhouse gas emissions, which is the main objective of the Paris Agreement (SOUSA, 2018).

Among the several energy matrices, which has been significantly studied. Bio fuels present an excellent proposal in their use, because they are biodegradable, and practically free of sulfur and aromatic compounds, with low emission rates of pollutants to the environment, becoming a promising alternative for the partial or total replacement of highly polluting fuels.

Among the various types of bio fuels, one of the main ones is ethanol. It can be obtained through sugarcane, corn, beet, manioc, potato, etc., the raw material is subjected to fermentation using the micro-organism Saccharomyces cerevisiae, obtaining a highly flammable and colorless fuel.

This alcoholic fermentation process is carried out in chemical reactors; in a general definition, a chemical reactor is a container where chemical reactions, mass and heat transfer occur. In chemical engineering, these reactors are vessels designed to contain chemical reactions of interest and industrial scale (CNTQ, 2013).

Due to the increased interest in the industrial application of alcoholic fermentation in chemical reactors, several kinetic models have been examined for cell growth, product formation and substrate consumption.

The creation of the kinetic model is one of the most important stages in the elaboration of a fermentation process, since these models help in the control of the fermentative process, obtaining fast and safe results without the realization of tests in a real plant, reducing process costs and increasing product quality (DODIĆ et al., 2012).

Kinetic models for industrial fermentations are usually based on simple and unstructured models, therefore not every kinetic model can be applicable in a real situation directly, thus starting from a simple model occurring adjustments of the parameters based on the system response to disturbances, until eventually reaching an adequate kinetic model (BIROL et al., 1998).

Since the models are defined, they can be used to describe different process conditions such as temperature, pH, aeration and mixing. This information allows us to design and control the fermentation process (DODIĆ et al., 2012)

2 Fermentative Kinetics

Knowing what is a factor of microbial growth, its proliferation mechanisms and the elements that influence is necessary to understand how they develop and their characteristics, thus enabling the control of this growth, the most important factor being the increase in the number of micro-organisms, that is, the increase in the number of cells in the population. Concerning the speed of growth, these microorganisms grow exponentially, which results in a rapid increase in the population. Because they are exponential, they have mathematical functions that describe the growth of the community, and each function differs for each distinct microorganism (VERNIER, 2020).

2.1 The growth model of Monod

In 1949, Jacques Monod (MONOD, 1949) presented a model responsibles for microbial growth parameters in aqueous environments with nutrient-limiting concentrations (VERNIER, 2020). This model presents the specific velocity as dependent on the growing concentration of bacteria as a function of the concentration of a single limiting substrate in the medium (S) in the case of ethanol production the sucrose concentration (MONOD, 1949).

As pointed out by (VERNIER, 2020) the Monod equation is based on the observation of the nonlinear relationship between substrate concentration and microbial growth, resulting in the specific growth rate of the microbial concentration as a function of the concentration of the limiting substrate and the saturation constant:

$$\mu = \mu_{max} \frac{S}{K_S + S} \tag{1}$$

2.2 Chemical reactors

The alcoholic fermentation process is carried out in chemical reactors; in a general definition, a chemical reactor is a container where chemical reactions, mass, and heat transfer occur. In chemical engineering, these reactors are vessels designed to contain chemical reactions of interest and industrial scale (CNTQ, 2013).

[4], defines chemical reactors as equipment where reactions occur for the transformation of raw materials into marketable products, with equipment of all shapes and sizes. The most common reactors are batch (BR), tubular (PFR), and continuous tank (CSTR).

In the batch reactor, its use is focused on small-scale operations, possessing the advantage of high conversions that can be obtained by leaving the reagent in the reactor for a long period, but it has high operating costs and large-scale production difficulties (FOGLER, 2009).

2.3 Mathematical model

To understand the kinetics of the alcoholic fermentation process using the micro-organism Saccharomyces cerevisiae, we need to calculate the biomass variation, substrate variation and product variation within a bioreactor. The equation of the biomass variation is obtained by correlating the equation describing the design of a chemical reactor, in this case the batch reactor, the equation describing the cell growth and the specific speed of this growth. Liu (LIU, 2020) defines the biomass variation equation, such as:

$$\frac{dX}{dt} = \mu X = \mu_{max} \frac{S}{K_S + S} X \tag{2}$$

and the change in substrate mass is given by:

$$\frac{dS}{dt} = -\frac{\mu_G X}{YF_{X/S}} = -\frac{\mu_{max} S}{K_S + S} \frac{X}{YF_{X/S}} \tag{3}$$

where:
S= substrate concentration;
X= cell biomass concentration;
$YF_{X/S}$ = yield factor;
μ_{max}= maximum growth rate;
μ_G=specific growth rate;
K_S= saturation constant.

3 Fractional calculus

Defitinion 1 (Riemann-Liouville) *The Riemann–Liouville fractional integral of $y(t)$ with order $\alpha > 0$ is given by the expression:*

$$\mathcal{I}^{\alpha} y(t) = \frac{1}{\Gamma(\alpha)} \int_0^t (t-s)^{\alpha-1} y(s) ds \tag{4}$$

Defitinion 2 (Caputo derivative) *The Caputo fractional derivative of $y(t)$ with order $0 < \alpha < 1$ is given by:*

$${}^{C}\mathcal{D}^{\alpha} y(t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t (t-s)^{-\alpha} y'(s) ds \tag{5}$$

The discretization of the fractional operators are given by (LI; ZENG, 2015):

$$\mathcal{I}^{\alpha} y_n \approx \widehat{\mathcal{I}}^{\alpha} y_n \tag{6}$$

$${}^{C}\mathcal{D}^{\alpha} y_n \approx {}^{C}\widehat{\mathcal{D}}^{\alpha} y_n, \tag{7}$$

in which $y_n := y(t_n)$, $t_n = nh$, $h > 0$ and the discretizations $\widehat{\mathcal{I}}^{\alpha}$ and $\widehat{\mathcal{D}}^{\alpha}$ are defined by

$$\widehat{\mathcal{I}}^{\alpha} y_n = \frac{h^{\alpha}}{\Gamma(1+\alpha)} \sum_{i=0}^{n-1} b_{n-i}(\alpha) y_{i+1} \tag{8}$$

$$\widehat{\mathcal{D}}^{\alpha} y_n = \frac{h^{-\alpha}}{\Gamma(2-\alpha)} \sum_{i=0}^{n-1} b_{n-i}(1-\alpha)(y_{i+1} - y_i), \tag{9}$$

with weights

$$b_j(\beta) = (j+1)^{\beta} - j^{\beta}. \tag{10}$$

4 Fractional model

Based on Caputo fractional derivative, we propose the following fractional derivative:

$${}^{C}\mathcal{D}^{\alpha} X = \mu X = \mu_{max} \frac{S}{K_S + S} X \tag{11}$$

and the change in substrate mass is given by:

$${}^{C}\mathcal{D}^{\alpha} S = -\frac{\mu_G X}{Y F_{X/S}} = -\frac{\mu_{max} S}{K_S + S} \frac{X}{Y F_{X/S}} \tag{12}$$

An alternative to equations Eq. (11) and Eq. (12) is the use of the discrete form to numerical implementation that is given by:

$${}^{C}\widehat{\mathcal{D}}^{\alpha} X_n = \mu_{max} \frac{S_{n-1}}{K_S + S_{n-1}} X_{n-1} \tag{13}$$

and

$${}^{C}\widehat{\mathcal{D}}^{\alpha} S_n = -\frac{\mu_{max} S_{n-1}}{K_S + S_{n-1}} \frac{X_{n-1}}{Y F_{X/S}} \tag{14}$$

The nonlinear problem is solved using numerical solutions to equations Eq. (13) and Eq. (14). These are expressed in the figures:

5 Numerical implementation

In this section, we compare the fractional and integer-order models, where we consider some values for α. This comparative analysis allows us to observe the different stabilization times of the chemical reactions that are occurring, with the simple change in the value of the parameter α. The parameters used are: $\Delta t = 0.1$, $\mu_{max} = 0.0974/h$, $K_S = 43.76g/L$, and $YF_{X/S} = 0.4036$. Add, we consider the initial data $X_0 = 1g/L$ and $S_0 = 50g/L$.

The programming language used was the Python language in its version 3.10, using the Pycharm IDE. The results obtained are extremely important since we can associate the fermentation time with α. We emphasize that we are working with a system of non-linear equations and therefore the use of discrete models is necessary to obtain the solutions. After the application of the fractional derivative in Equations 2 and 3, which describes the variation of biomass and substrate, respectively, we can observe the performance of the estimate, according to the variation of each α used:

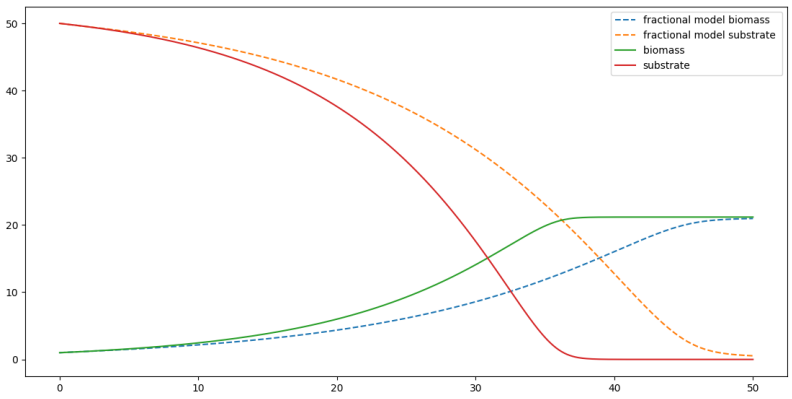

Figure 1: Fractional model with $\alpha = 0.9$

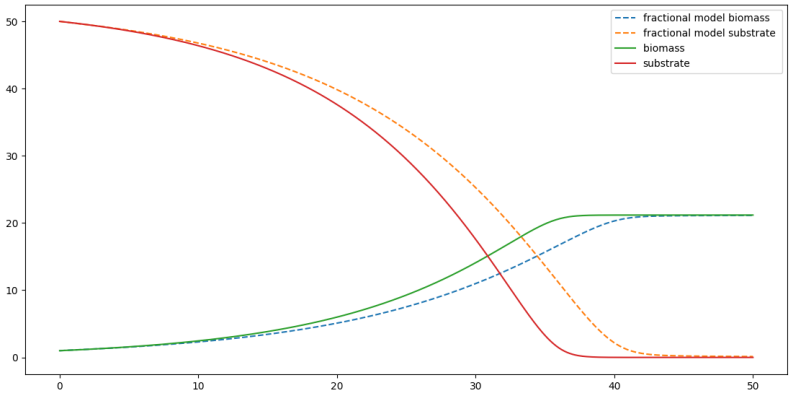

Figure 2: Fractional model with $\alpha = 0.95$

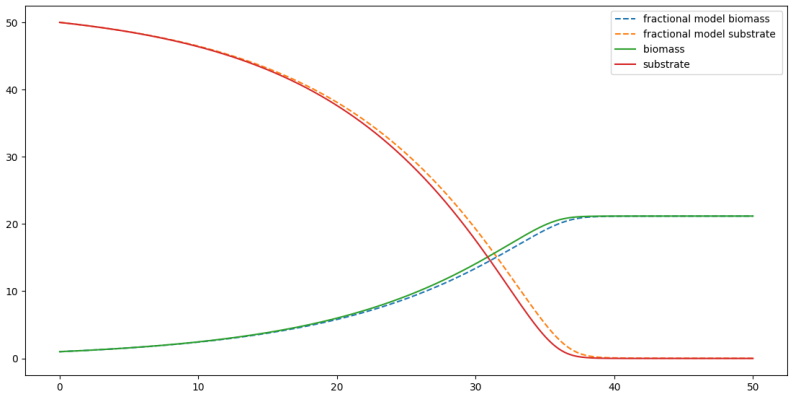

Figure 3: Fractional model with $\alpha = 0.99$

6 Considerations

In this work, a mathematical method was used to estimate the solution of the Monod model for fermentative growth of the microorganism Saccharomyces cerevisiae. The proposed model is based on the use of Caputo fractional derivative applied to the Monod equation. Providing variations in numerical solutions of the whole order, both for the substrate and for biomass. It is important to note that the fractional case recovers the entire order solution when $\alpha \rightarrow 1$.

References

BIROL, G. et al. Mathematical description of ethanol fermentation by immobilised saccharomyces cerevisiae. **Process Biochemistry**, Amsterdam, v. 33, n. 7, p. 763–771, 1998.

CNTQ. Reator Químico. Confederação Nacional dos Trabalhadores no Ramo Químico, 2013. Disponível em: <http://cntq.org.br/wp-content/uploads/2013/05/Reator-quimico.pdf>. Acesso em: 24 ago. 2021.

DODIĆ, J. M. et al. Kinetic modelling of batch ethanol production from sugar beet raw juice. **Applied energy**, Elsevier, v. 99, p. 192–197, 2012.

FOGLER, H. S. **Elementos de engenharia das reações químicas**: comsol multiphysics. Rio de Janeiro: LTC-Livros Tecnicos E Cientificos, 2009.

LI, C.; ZENG, F. **Numerical methods for fractional calculus**. [S.l.]: CRC Press, 2015. v. 24.

LIU, S. **Bioprocess engineering**: kinetics, sustainability, and reactor design. [S.l.]: Amsterdam, 2020.

MONOD, J. The growth of bacterial cultures. **Annual review of microbiology**, Annual Reviews 4139 El Camino Way, v. 3, n. 1, p. 371–394, 1949.

SATO, I.; ELLIOT, B.; SCHUMER, C. **O que é uma economia dependente de carbono e como evitá-la?** WRI BRASIL. São Paulo: [s.n.], 2021. Disponível em: <https://wribrasil.org.br/pt/blog/clima/o-que-e-uma-economia-dependente-de-carbono-e-como-evita-la>. Acesso em: 24 nov. 2021.

SOUSA, R. **Acordo de Paris**. Brasil Escola. 2018. Disponível em: <https://brasilescola.uol.com.br/geografia/acordo-paris.htm>. Acesso em: 24 nov. 2021.

VERNIER, P. **Crescimento microbiano**. FEAGRI. 2020. Disponível em: <https://wiki.feagri.unicamp.br/doku.php?id=fa733:crescimentoicrobiano>. Acesso em: 18 nov. 2021.