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Research Article

Application of the ABC Algorithm in Parameter Estimation and Kinetic Model Selection in Propionic Fermentation

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ABSTRACT

A propionic acid fermentation process not only provides a more sustainable approach, but also opens the door to propionic acid production capacity in regions with limited petroleum supplies. With fermentation, low-cost substrates can be used, such as residual biomass; reducing their concentration in nature. This process becomes interesting because from it propionic acid is considered natural. Several models have already been developed to describe the dynamics of components such as: Microorganism (biomass), nutrients (substrate), metabolites (product). However, a challenge is how to define the model that best represents the kinetic term, and therefore, there are several models for this modeling. This article's novelty is the application of the Bayesian technique (Computational Bayesian Approximation) to estimate parameters and simultaneously select the best model. Model validation was carried out considering propionic fermentation regarding experimental data from the literature which one was selected the Andrews model as the best to predict the dynamic of biomass, substrate and product been the following parameters estimated μ_{max}= 0.192, ms = 0.005, mp = 0.017.

1. Introduction

Propionic acid, with the molecular formula $C_3H_6O_2$, is a colorless substance with a strong odor. This short-chain fatty acid has various applications, such as a preservative in animal feed, dairy products, and baked goods. Additionally, it is used as a chemical intermediate in the production of pharmaceuticals, herbicides, cosmetics, and cellulose acetate[1-2].

Although the chemical synthesis of propionic acid is economically viable, petroleum, a finite resource, faces increasing challenges and restrictions, such as limited access and a lack of complex catalysts. Due to pollution caused by non-renewable sources, many studies aim to improve the sustainable production of propionic acid, including alternatives like fermentation. [3-4].

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A propionic acid fermentation process not only provides a more sustainable approach, but also opens the door to propionic acid production capacity in regions with limited petroleum supplies. With fermentation, low-cost substrates can be used, such as residual biomass; reducing their concentration in nature. This process becomes interesting because from it propionic acid is considered natural[1-4]

Initially, the kinetic study of a dynamic fermentation process involves analyzing the concentration evolution of one or more components of a system. It comprises components: Microorganism (biomass), nutrients (substrate), metabolites (product). Which are generally represented by X, S and P in mathematical models [5].

A tool that contributes to the advancement of the process is the development and application of mathematical models. In mathematical modeling of the fermentation process, it is necessary to determine the kinetic model that represents the process [6]. Kinetic models indicate how the variables under study affect the speed of cell growth, product generation and substrate consumption.

The choice of kinetic model varies according to the type of process being worked on, such as in [7], where the Anaerobic Digestion Model No. 1 (ADM1) is modified to simulate biogas production in a large-scale agricultural plant by dividing carbohydrates into starch, cellulose, and hemicelluloses, and proteins into rapidly and slowly degrading fractions. Lactic acid was also added to the model. The model calibration was carried out in several stages: initial selection of coefficients based on the literature, sensitivity analysis to identify important parameters, and determination of the final parameter values, ensuring accuracy within a 95% confidence interval. The article aims to improve ADM1 for more accurate and relevant simulations of biogas production in agricultural contexts.

In another approach, still concerning anaerobic digestion, [8] describes pressurized anaerobic digestion as an effective method for producing biogas with high methane content, reducing the costs of upgrading and injecting biogas into the distribution network. This process has attracted scientific interest in the last decade, leading to the development of kinetic models for its optimization. The mentioned work proposes a modified model, model n.1, which analyzes the autogenerative high-pressure anaerobic digestion of volatile fatty acids in a batch system, evaluating the impact of the increased autogenic pressure in the reactor on the efficiency and dynamics of biogas production.

In this work, three kinetic models described in the literature were analyzed: Monod, Andrews and Alba. Where each model presents different hypotheses to make inferences about the analyzed process.

The mathematical models are composed of the initial biomass value (X), substrate-to-product conversion factor (Yp/s), substrate-to-cell conversion factor (Yx/s), cell maintenance coefficient (ms), coefficient product mass (mp) and specific cell growth speed (μx). However, in order to have the complete model, it is still necessary to have a function for μx (kinetic model). Kinetic models are generally represented by a system of ordinary, coupled differential equations that describe reactions and interactions between reaction elements [9-10].

In this sense, with the intention of determining which model best represents the phenomenon studied, we chose to use the Bayesian technique Approximate Bayesian Computation (ABC), since this technique, in addition to estimating parameters, simultaneously selects the best model.

2. Fermentation Kinetic Models

The mathematical modeling and parameters of the fermentation process were based on [11]. This is a kinetic evaluation and mathematical modeling in propionic fermentation. The materials used in the system were: analytical grade glycerin (P.A. CHEMCO) as the carbon source and the microorganism *Propionibacterium acidipropionici* CCTT4843 (NRRL B-3569) for the fermentations. The concentration measurements were performed using gravimetry (dry weight), and the concentrations of organic acids and glycerol were determined by high-performance liquid chromatography (HPLC). The process occurred in batch mode, meaning that all the substrate was added at the beginning and no reagents were added to the system, except for those used for process control and safety. The kinetics of a bioprocess consists of analyzing the evolution of concentration values of one or more components of the production system, as a function of the time of the bioprocess. The mathematical model uses mass balances to describe growth kinetics, substrate consumption and product production. The unstructured substrate, biomass and product models are presented in Eqs (1.a-c):

$$\frac{dS}{dt} = -\left(\frac{\mu_X}{Y_{X/S}} + m_s\right).X \tag{1.a}$$

$$\frac{dX}{dt} = \mu_X X \tag{1.b}$$

$$\frac{dP}{dt} = \mu_X.Y_{P/X}.X + m_p.X \tag{1.c}$$

where μ_X is the specific cell growth rate; $Y_{X/s}$ is the substrate-to-cell conversion factor; m_s is the cell maintenance coefficient; $Y_{P/X}$ is the product yield factor in relation to biomass; m_p is the mass coefficient of the product.

The models evaluated differ in the way they represent the specific speed (μ_x). Below are some formulations for μ_x.

Monod.

The simplest kinetic model is the Monod model (eq. 2a). This model presents the specific speed as dependent on the limiting substrate concentration in the medium (S).

$$\mu_x = \mu_m \frac{S}{K_S+S} \qquad (2.a)$$

where μ_m (h^{-1}) is the maximum cell growth speed, Ks (g.L $^{-1}$) is the saturation constant

The constant Ks is known as Monod's constant and represents the substrate concentration at which the growth rate is half the maximum speed [12]. The Monod model is a simplification of the complicated mechanism of cell growth. This model does not consider the inhibition effect due to substrate and product concentrations; it only considers the substrate as limiting.

Andrews.

At high substrate concentrations, cell growth can be inhibited. Aiming to represent the inhibition effect [13] proposed Eq. 2.b. In this model, in addition to considering the substrate as limiting, it also considers it as an inhibitor.

$$\mu_x = \frac{\mu_m S}{K_S+S+\frac{S^2}{K_i}} \qquad (2.b)$$

where Ki (g.L $^{-1}$) is substrate inhibition constant

When the substrate concentration (S) is lower than the value of the constant Ki, the value of the inhibition term (S2 /Ki) tends to zero. Therefore, there is no influence of the term on the value of microbial kinetics. When the inhibition term is nullified, the Andrews model is reduced to the Monod model.

Alba.

In this model, inhibition without product competition is considered.

$$\mu_x = \frac{\mu_m}{(1+\frac{K_S}{S})(1+\frac{P}{Kp})} \qquad (2.c)$$

The phenomenon of cell growth inhibition only applies to relatively low S values, less than or equal to Ks.

3. Computational Bayesian Approximation

In several scenarios in mathematical modeling there are difficulties in determining unknown parameters that in some models cannot be determined directly or the experiment to determine them is expensive [14-19]. One of the solutions to this difficulty is to perform inference through statistical techniques.

Among the classical statistical techniques, the most widespread is the least squares method, while among the Bayesian techniques, the most used are Maximum Likelihood and the Monte Carlo method via Markov Chain. Bayesian techniques are based on Bayes' theorem to make inferences [20-24].

$$\pi_{posteriori}(\theta|data)\ \alpha\ \pi_{priori}(\theta)L(data|\theta)(3)$$

where $\pi_{posteriori}(\theta|data)$ represents the posterior probability density of the parameters, $\pi_{priori}(\theta)$ prior probability distribution and $L(data|\theta)$ the likelihood function.

In some cases it is difficult to represent the likelihood function and in these cases it becomes unfeasible to use the Maximum Likelihood and Monte Carlo via Markov Chain methods. Because of this difficulty, the Computational Bayesian Approximation technique was used, since this technique does not require the Likelihood function to be represented.

Using the algorithm proposed by Toni et al. (2009)[25], the ABC technique uses transition populations to update the posterior probability distribution of the parameters referring to each model studied, in this way the posterior probability of each parameter is represented by the last population [26-25-30. However, one of the challenges of applying ABC lies in choosing the appropriate stopping criterion. Therefore, this work proposes an algorithm with stopping criteria based on the coefficient of variation (CV) of particle distances that were accepted in the previous population, as follows in Table 1.

Table 1: Modified ABC Algorithm.

1	Initialize with tolerance ε and high CV_1 coefficient of variation. Establish the limit value of the CV_{limit} coefficient of variation. Define the indicator population *pop = 0*.
2	Define the indicator particle *i = 1*
3	Sample the model m^* from the model prior $\pi(m)$. If *pop = 0*, draw the set of parameters $\boldsymbol{\theta}^*$ of model m^* independently of the prior parameters of the model drawn $\pi(\boldsymbol{\theta}(m^*))$. If

$pop > 0$, draw $\boldsymbol{\theta}^*$ of the previous population $\{\boldsymbol{\theta}(m^*)_{pop-1}\}$ with weight $w(m^*)_{pop-1}$ and move the particle $\boldsymbol{\theta}^*$ with a transition kernel (K_{pop}) para obter $\boldsymbol{\theta}^{**} \sim K_{pop}(\boldsymbol{\theta}/\boldsymbol{\theta}^*)$. If $\pi(\boldsymbol{\theta}^{**}) = 0$, return to step 3.

Simulate a set of candidate data from the posterior distribution: [S P X] $\sim \pi([S\ P\ X]\ /\boldsymbol{\theta}^{**}, m^*)$. If the distance function $d([S\ P\ X]^{exp}, [S\ P\ X]^*) \geq \varepsilon$, come back to step 3.

4 Define $m^{(i)}_{pop} = m^*$ and add $\boldsymbol{\theta}^{**}$ for the particle population $\{\boldsymbol{\theta}(m^*)_{pop}\}$ and calculate the weight of the particle $\boldsymbol{\theta}^{**} as$:

$$w^{(i)}_{pop} = \begin{cases} 1, & \text{if } p \\ \dfrac{\pi(\theta^{**})}{\sum_{j=1}^{N} w^{(j)}_{pop-1} K_{pop}\left(\theta^{(j)}_{pop-1} / \theta^{**}\right)} & \text{if } p \end{cases}$$

5 If $i < N$, define $i = i + 1$ and come back to step 3.

6 For each model m, normalize the weights of the accepted particles.

7 If $CV_{pop} > CV_{limit}$, define $pop = pop + 1$ and come back to step 2. Otherwise, stop.

4. Results

The application of the computational Bayesian technique (ABC) was carried out considering propionic fermentation data from [11]. The a priori probability distributions were considered to be a uniform distribution with the values presented in Table 2. Since it is a kinetic process, the distributions follow positive values, making them physically possible. High values for the parameters were considered to fit the hypotheses. The initial conditions used for biomass, substrate and product were X(0) = 0.10, S(0) = 20.00 and P(0) = 0.00 respectively (Marinho et al. 2018).

Table 2: Limits for the prior probability distribution (uniform distribution).

Monod		Alba		Andrews	
ms (h^{-1})	[0 1.00]	ms (h^{-1})	[0 1.00]	ms (h^{-1})	[0 1.00]
μ_{max} (h^{-1})	[0 1.00]	μ_{max} (h^{-1})	[0 1.00]	μ_{max} (h^{-1})	[0 1.00]
Ks (g/L)	[0 40.00]	Ks (g/L)	[0 20.00]	Ks (g/L)	[0 50.00]
mp (h^{-1})	[0 0.20]	Kp (g/L)	[0 76.00]	mp (h^{-1})	[0 0.30]
		mp (h^{-1})	[0. 0.30]	Ki (g/L)	[0 60.00]

By applying the Computational Bayesian Approximation Bayesian algorithm, considering the measurements of X, S and P presented by Marinho et al. 2018. The analyzes were carried out to verify whether the tolerance was monotonically decreasing (Figure 1), which model order best represents the experimental data (Figure 2), parameter estimates (Table 3) and analyze whether the models were able to simulate the experimental data by comparing the simulated and experimental data (Figure 3-5).

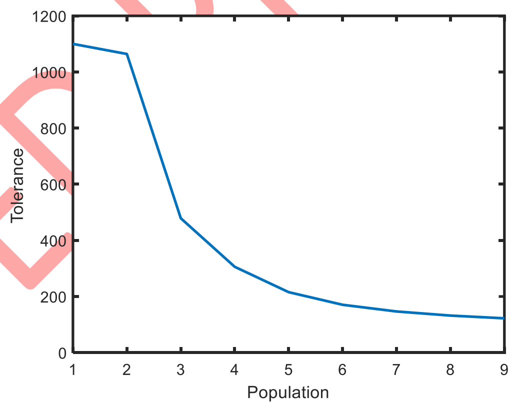

Figure 1: Tolerance in each population of the algorithm.

It can be seen in Figure 1 that tolerance satisfied the condition of being monotonically decreasing, observing that the greatest reduction was in the advancement from the second to the third population. However, the algorithm needed 9 populations to reach the adopted stopping criterion. (C.V. = 0.30).

The parameter estimates are presented in Table 2, the estimates were made by evaluating the samples of each parameter in the last population. With these samples, the mean and 99% credibility interval for X, S and P for each model are calculated.

Table 3: Parameter estimates (mean and 99% credibility interval).

Monod		Alba		Andrews	
ms (h^{-1})	0.007 (0.002; 0.103)	ms (h^{-1})	0.008 (0.005 ; 0.013)	ms (h^{-1})	0.005 (0.001 ; 0.0013)

μ_{max} (h^{-1})	0.112 (0.083 ; 0.214)	μ_{max} (h^{-1})	0.109 (0.099 ; 0.127)	μ_{max} (h^{-1})	0.192 (0.093; 0.229)
Ks (g/L)	16.146 (8.393 ; 44.874)	Ks (g/L)	13.251 (10.746; 18.189)	Ks (g/L)	22.912 (2.657 ; 54.887)
mp (h^{-1})	0.024 (0.004 ; 0.042)	Kp (g/L)	38.774 (27.869 ; 51.044)	mp (h^{-1})	0.026 (0.005 ; 0.052)
		mp (h^{-1})	0.017 (0.007 ; 0.028)	Ki (g/L)	27.27 (5.993 ; 72.42)

Where *ms* is the substrate maintenance rate, representing the minimum amount of substrate a microorganism needs to maintain its vital functions (cellular maintenance) without growing; *mp* is the specific production rate of the product, representing the rate at which a product (such as a metabolite) is formed per unit of biomass per unit of time; μmax is the maximum specific growth rate, representing the maximum growth rate of microorganisms when the substrate is in excess and other environmental conditions are ideal; *Ks* is the saturation constant (or affinity constant), representing the substrate concentration at which the growth rate is half of μmax. It indicates the affinity of microorganisms for the substrate.

These parameters are of fundamental importance as they improve fermentative processes in terms of efficiency and productivity, as well as help in monitoring and controlling the process, allowing real-time adjustments to maintain ideal conditions. Substrate optimization helps determine the ideal amount of substrate to be used, minimizing waste and maximizing microbial growth and metabolite production. They are fundamental for the planning of new fermentative processes and the improvement of existing processes, ensuring scalability and economic viability [12; 31-32].

When evaluating Table 2, it is clear that the parameters in common between the models (ms; μ_{max}; Ks and mp) present estimates of the same magnitude. This assessment of the credibility of the estimate by having the same physical meanings. It can be concluded that the methodology has good precision when verifying that the range of the credibility interval is small when compared with the average of the estimates. However, it can be seen that the smallest range is precisely that of the Andrews model, which was selected as the best (see Figure 2), as it has a higher frequency in the last population to be evaluated (ninth population).

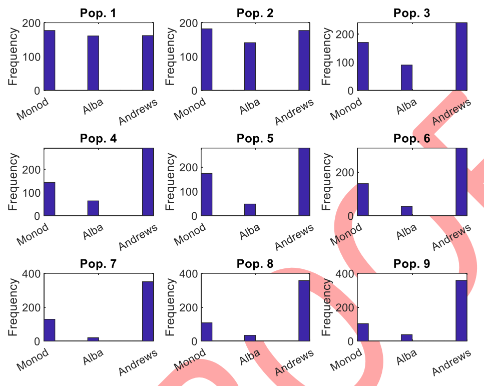

Figure 2: model selection according to population evolution.

Finally, comparisons between the estimates of X, S and P with the experimental measurements were evaluated considering the 3 kinetic models. These comparisons are presented in Figures 3-5.

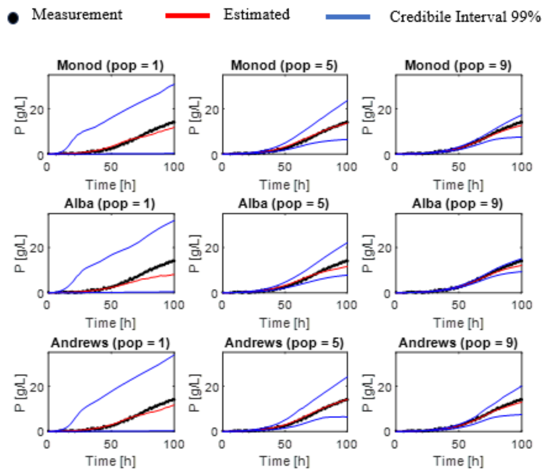

Figure 3: Comparison between simulated and experimental measurements of product P.

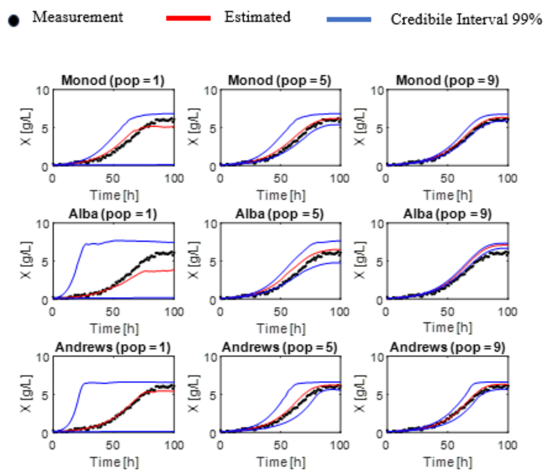

Figure 4: Comparison between simulated and experimental measurements of biomass X.

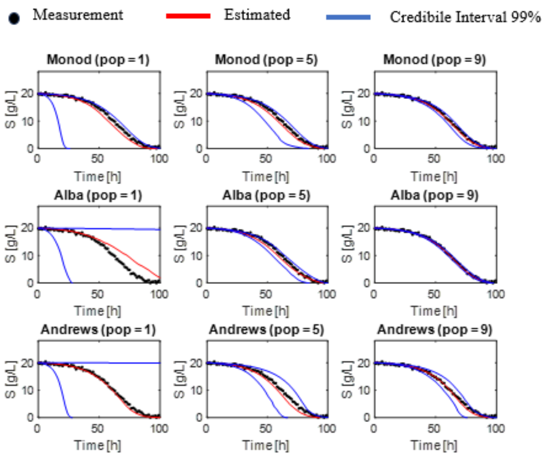

Figure 5: Comparison between simulated and experimental measurements of substrate S.

Figures 3-5 present the estimates of the product P, substrate S and biomass X. It can be seen that in the first population in all state variables (P, S and X). This happens because in the first population the parameter samples are randomly drawn from the a priori probability distribution. As the populations advance, the parameter space of the parameters reduces and consequently the uncertainty of the state variables (P, S and X) reduces, as can be seen in Figures 3-5 when comparing the uncertainties in populations 1, 5 and 9.

It is observed in Figures 3-5 that the Andrews model has a slightly slower kinetics compared to the other models. This effect occurs due to the presence of the inhibition factor by the substrate (Ks) and by the product (Ki), which slow down the cell growth rate. It is also noted that all substrate was consumed and the models predict the same amount of product formed. Therefore, using the Andrews model, there is no possibility of total inhibition due to the substrate concentration (µx = 0). This model implies that cells are capable of growing regardless of the substrate concentration in the medium, which is contrary to what is observed in reality. There is a concentration at which cell growth is completely inhibited (MULCHANDANI & LUONG, 1989).

5. Conclusions

The Bayesian technique Computational Bayesian Approximation proved to be robust and capable of estimating parameters and selecting models simultaneously in kinetic models applied to simulate the dynamics of substrate S, product P and biomass X. When applied to propionic fermentation data, the algorithm selected as the best model which represents the kinetics by the Alba equation been the parameters estimated μ_{max}= 0.192, ms = 0.005, mp = 0.017. In addition to this being the best model, it was verified that this model represents very well the dynamics of the state variables (S, P and X). Therefore, if to wish to simulate propionic fermentation in different scenarios, can use the system of coupled ordinary differential equations presented and considering the Andrews kinetic model with the estimated parameters.

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Conflicts of Interest

Authors must disclose all potential conflicts of interest in the manuscript, including financial, consultant, institutional and other relationships that might lead to bias or a conflict of interest. If there is no conflict of interest it should be stated as: The author declares that there is no conflict of interest regarding the publication of this article.

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