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Modeling Of the Kinetics of Ethanol Formation from Glucose Biomass in Batch Culture with a Non Structured Model

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ABSTRACT

A mathematical modeling of the batch fermentation kinetics of a novel thermotolerant strain of the yeast Kluveromyces Maxianus evaluated at 40^{0}C. Non-structured models were used to describe the experimental data. Different biological models were test with the experimental data. Logistics model fitted to the glucose biomass production with a R Square value of 0.97 and modified Gompertz model can be said to successfully describe the kinetics of ethanol production with a value of 0.996. Mathematical models are becoming more relevance in biological process and microbial growth. Model gives more insight into the environmental conditions surrounding bio-process and can be used for further development and optimization of bio-processes.

Keywords

I. INTRODUCTION

Sugar feedstocks are biomass materials containing high levels of glucose or precursors to glucose. They are the easiest feedstock to be converted to ethanol. An example of a sugar feedstock is sugarcane. Brazil developed a successful fuel ethanol program from sugarcane because of high yields of sugarcane in the country [1,2,3].

Fungi, bacteria, and yeast microorganisms can be used for the fermentation, specific yeast like *maxianus kluveromyces, Saccharomyces cerevisiae* can be used to ferment glucose to ethanol.

Considering the growing interest of researchers and great economic potential of ethanol as an alternative to fossil fuels, fermentation technology must take care for several variables involved in the production of ethanol to optimize the productivity of the process [4]. Variables like biomass resources, microorganisms, simultaneous sacharification and fermentation (SSF), agitation speed, substrate composition, reaction time and pH of the culture medium should be controlled to produce optimum results. This brings to bear the use of models as a mean of optimization with less experimental work.

Mathematical models are a means of representing essential aspects of reality with the help of symbols, number and functions etc. Mathematical models typically offer convenience and cost advantages over other means of obtaining the required information on reality. In the last decades, continuing progress has been observed in applications of mathematical modeling in biological growth. A great deal can be learned about the real life phenomenon by manipulating a model's variables and observing the results once models are developed properly [5].

In developing fermentation process, Kinetic modeling has been regarded as an important step since models help in both process control and research efforts, where they will be most effective in reducing process costs and increasing product quality [6]. With increasing interest in the industrial application of batch alcoholic fermentation, various kinetic models have been proposed for microbial growth, product formation, and substrate consumption [7].

Both structured and unstructured have been proposed, while structured models can explain complex microbial systems at molecular levels, relatively simpler non-structured kinetic models have frequently been used for practical applications [8, 9]. Once these models are robust, they can be used to describe the production processes under different process conditions, such as temperature, pH, aeration and mixing, among others [6]. Having achieved efficient numerical models, production designs and processes can be adequately understood and controlled for optimum results.

A number of studies have been done on kinetic modeling of ethanol as regards its fermentation time. However, only few modeling has been done to date on the production of ethanol through batch fermentation of glucose biomass with a thermotelerant strain of *Kluveromyces Maxianus*, this research adopted the experimental result of the This research is a step ahead on biological growth modeling as it describes the kinetics of ethanol fermentation with a set of unstructured model incorporating varying fermentation time from (0 – 30h) at an elevated temperature of 40^{0}C.

II. MATERIALS AND METHOD

2.1 Experimental Data Source

The experimental data utilized by this study was the batch fermentation kinetics of a novel thermotolerant strain of the yeast *Kluveromyces Marxianus* evaluated 40°C by [10](Hughes, *et al.*, 1984). Several strain of this species have received attention for their mesophilic yeast temperatures (30 – 35), however, isolated strain of *Kluveromyces Maxianus* capable of ethanolic fermentation at temperature above those previously reported for yeast was understudied.

2.2 Mathematical Models

There are basic biological models that can be used to describe biochemical processes successfully. The experimental data were subjected to different kinetics models and the model that best fit the experimental data was adopted. These models are shown in Table 1.

TABLE 1. SOME BIOLOGICAL MODELS

S/N	Name	Model
1	Logistic Model	$y = \frac{a}{1+\exp(b-cx)}$
2	Gompertz Model	$y = a.\exp[-\exp(b-cx)]$
3	Modified Gompertz Model	$y = a\,exp\left\{-exp\left[\frac{\mu_m \exp(1)}{a}(\lambda - t) + 1\right]\right\}$
4	Richards Model	$y = a\{1 + v.\exp[k(\tau - x)]\}^{\left(-\frac{1}{v}\right)}$
5	Stannard Model	$y = a\left\{1 + exp\left[-\frac{(l+kx)}{P}\right]\right\}^{(-\sigma)}$
8	Schnute Model	$y = \left\{y_1^b + (y_2^b - y_1^b).\frac{1-\exp[-a(t-\tau_1)]}{1-\exp[-a(\tau_2-\tau_1)]}\right\}^{1/b}$

[Source:11]

It was found that Logistic model describes the kinetic of glucose biomass growth and modified Gompertz equation can successfully describe the kinetics of ethanol mass concentration with respect to fermentation time at the experimented temperature.

2.2.1 Biomass Kinetic Growth Model

A non structured, sigmoidal shaped model, especially logistic model is widely used to describe microbial growth. Quite a number of polysaccharide fermentation processes and biomass growth have been described by logistic equation.

Under optimal growth condition and when the inhibitory effects of substrate and product were neglected, the rate of cell growth follows the well-known exponential relation as expressed in equation (1).

$$\frac{dX}{dt} = X\mu_m \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (1)$$

Where, μ_m (h^{-1}) is maximum specific growth rate of cells in time (t), with respect to the fermentation conditions,

X is biomass concentration (g/l) and;

t is the time.

The equation above means that X increases with time regardless of substrate availability. In real life, the given hyperbolic relationship governs the growth of cell is given by equation (2) below.

$$\frac{dX}{dt} = \mu_m X\left[1 - \frac{X}{X_m}\right] \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (2)$$

Where X_m is the maximum biomass concentration in $g.l^{-1}$ and,

X_0 is the minimum or initial biomass concentration in gl^{-1}.

This equation is known as the Riccati equation (11Mohammad *et al.*,2008), using the boundary condition at $t=0$ then $X = X_0$, gives a sigmoidal variation of X as a function of time. Equation (2) can be easily integrated to give the logistic equation which may represent both an exponential and a stationary phase. The resulted equation is shown in equation (3)

$$X = \frac{X_m X_0 e^{\mu_m t}}{X_m - X_0 + X_0 e^{\mu_m t}} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (3)$$

further simplification gives equation (4)*and* (5):

$$X = \frac{X_m X_0 e^{\mu_m t}}{X_m - X_0 + X_0 e^{\mu_m t}} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (4)$$

$$X = \frac{X_0 e^{\mu_m t}}{1 - \frac{X_0}{X_m} 1 - e^{\mu_m t}} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (5)$$

The equation (5) above is generally known as logistic equation which can accurately describe the kinetics biomass growth with time. It may represent both an exponential and stationary phase, however, the logistic equation presented above, does not predict the death phase of microorganisms after the stationary phase.

2.2.2 Ethanol Concentration Model

The modified Gompertz model can successfully describe the data of the fermentative production of ethanol from glucose biomass using a theremotolerant strain of *kluveromyces Maxianus*.

The double exponential Gompertz function Model is written as:

$$y = a.\exp[-\exp(b-cx)] \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (6)$$

After modification, modified Gompertz model can be written as:

$$y = a\,exp\left\{-exp\left[\frac{\mu_m \exp(1)}{a}(\lambda - t) + 1\right]\right\} \ldots\ldots\ldots\ldots\ldots (7)$$

The kinetic parameters are:

y = the ethanol mass concentration (g/L),

a = the potential maximum ethanol mass concentration (g/L),

μ_m = the maximum ethanol production rate ($gl^{-1}h^{-1}$),

λ = the lag phase or the lag phase or the time to exponential ethanol production (h).

t = fermentation time.

Equation (7) can be written as:

$$A_{EtoH} = A_m\,exp\left\{-exp\left[\frac{Pr_m \exp(1)}{A_m}(\lambda - t) + 1\right]\right\} \ldots\ldots (8)$$

Where:

A_{EtoH} = the ethanol mass concentration (g/L),

A_m = the potential maximum ethanol mass concentration (g/L),

Pr_m =the maximum ethanol production rate ($gl^{-1}h^{-1}$), or productivity

III. RESULTS AND DISCUSSION

3.1 Kinetics of Biomass Growth

The experimental data of the kinetic of the biomass growth were adopted and these experimental data were subjected into logistic model and the result was plotted and compared with experimental data. Fig 1 shows the comparison of both the experimental data and the logistic model. Logistic model successfully describe the experimental data of the biomass growth with time. The R square of this model shows a high value of 0.97, this show a significant correlation between the experimental data and model, which mean logistic model is well able to describe the kinetics of the biomass growth.

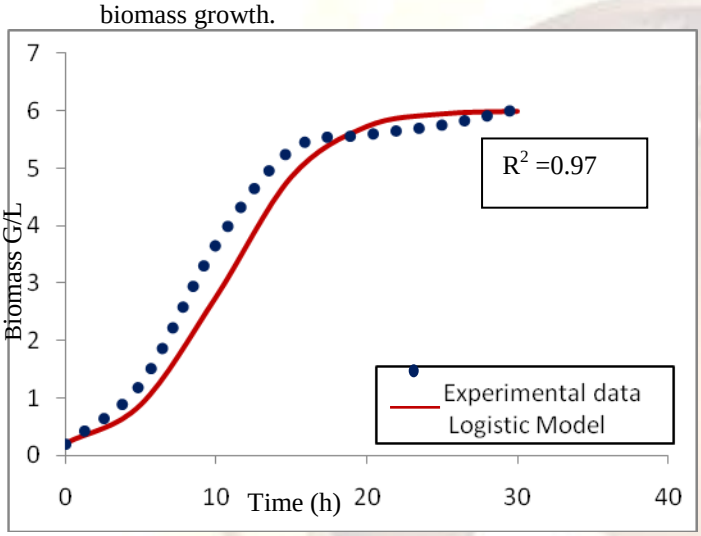

Figure 1. Result of Logistics Model

3.2 Ethanol Mass Concentration Result

The kinetic parameters of the ethanol mass concentration of the experimental data were adopted and subjected to modified Gompertz model and the result was plotted alongside with the real life experimental data as shown in Fig 2. Both of the results show high level significance of correlation with an R square value of 0.996. The high value of the R square suggests that the modified Gompertz model can be successfully use to describe the fermentation process for the production of ethanol from glucose biomass. This was also verified in the study on kefir grain fermentation for the purpose of ethanol production [13,14.]

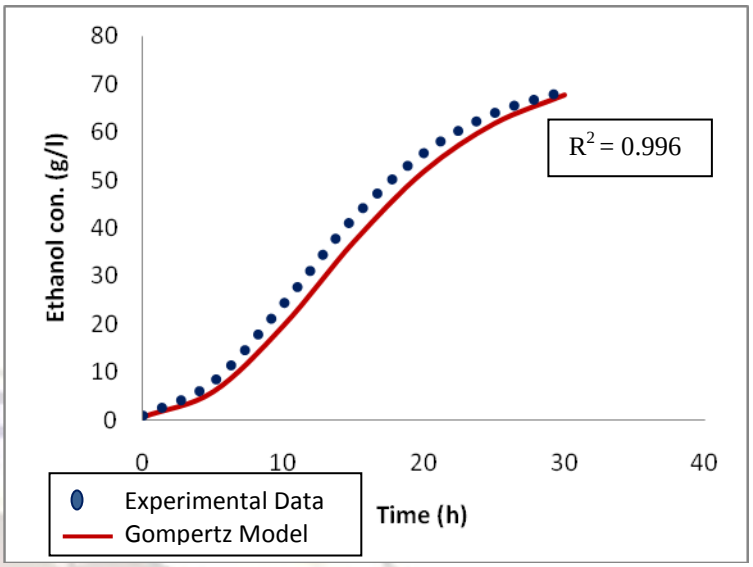

Figure 2. Result of Modified Gompertz Model

IV. CONCLUSION

Logistics model was used to illustrate the kinetics of biomass production with respect to time and modified Gompertz model was used to test the kinetics of ethanol mass concentration production at an operating temperature of 40^0C. Logistics model was well fitted to the experimental data with a R square value of 0.97 and could be regarded as sufficient to describe the biomass production. Also, the modified Gompertz model fitted into the experimental data and can also be regarded as sufficient to illustrate the fermentation process for the production of ethanol from glucose biomass with a novel thermotolerant strain of Kluveromyces Maxianus.

Comparing experimental and mathematical modeling, results shows no significant difference, therefore, utilization of mathematical model will contribute to a better understanding of effects of various factors affecting the production of ethanol. In other word, models enable us to understand, design, and control the fermentation process better and can be also be used for further process development.

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