MATHEMATICAL MODELING FOR ETHANOL PRODUCTION FROM MOLASSES USING THERMOTOLERANT *Kluyeromyces Marxians*

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ABSTRACT *Due to rapid depletion of fossil fuel reservoirs there is a need of identifying and extraction of new sources of energy. Bioethanol is known as future fuel that fulfills the requirement of petroleum based fuels. Bioethanol can be used as a base fuel or blended with gasoline used in vehicles without polluting the environment. Mathematical modeling plays an important role to understand the fundamental relationship between different variables and give an economic way to optimize various parameters. Monod Model gave a fundamental kinetic relationship between the production rates versus time. The main purpose of this paper is to derive the mathematical models for the rate of the cell mass, production and substrate consumption from the Monod model. The experimental data has been used to develop the models. The ODE45 package in Mat Lab has used to solve the differential equations. The model has been validated against the experimental results and found data in good agreement.*

Keywords: Monod model, Ethanol, Molasses, *kluyeromyces marxianus*, Mathematical modeling

INTRODUCTION

With the requirement of energy overall world increasing, new renewable energy required to be investigating and modified the production in order to meet the future requirement of energy. Mathematical modeling is also getting interest regarding development in any system for optimization [2]. Ethanol batch fermentation of *Saccharomyces cerevisiae* revealed that lower culture temperatures caused slower growth and slower ethanol production, however, the final cell mass and ethanol concentrations reached levels which were higher than those for higher culture temperatures [1]. To enhance the productivity of the alcohol fermentation process, combined aerobic and anaerobic fed batch operation could improve the growth of microbes and also achieve better alcohol production because of well-utilizing the characteristics of the microbial metabolism [3]. Using a realistic model fitted from experimental data, result shows that the highest productivity can be achieved using a proposed fed-batch operation with high glucose concentration, mathematical model were developed to see the effects of temperature on ethanol production using *saccharomyces cerevisiae* as yeast using cane molasses as the substrate [4]. Three state variables, biomass, ethanol and the substrate and kinetics parameters were used to describe the phenomenon [5]. The integrated Monod and Haldane models were used to evaluate the kinetic coefficients and their standard deviations using the methane accumulation curves of low-temperature *acetoclastic methanogenesis* [6]. For scale up any process kinetic parameter is very much important as for fermentation process were involved. The optimal values of the kinetic parameters were determined by fitting the models into the experimental data i.e. by minimizing the discrepancy between the model predictions and corresponding experimental data. The growth of yeast cells could be expressed by a logistic function model, which describes the growth as a function of initial biomass concentration, fermentation time, specific growth rate and final biomass concentrations [7].

MATERIALS AND METHOD

Materials

Strain of ther motolerant *Kluyveromyces marxianus* M15 were used in microprocessor controlled 23-L stainless steel fermenter.

Methodology

Monod model kinetics had been validated using experimental data from previous work, the method that will follow for validate the Monod model are given in Fig. 1.

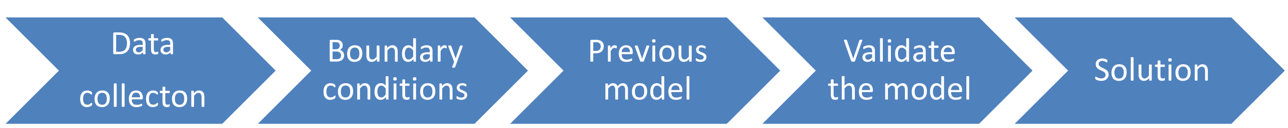


Fig. 1: Methodology for Validate the Previous Model

Data were collected from previous research work ,on the basis of that model is validated .During the process of fermentation, some factor is involved , these factor must be corrected in model to satisfy the experimental work.

Data Collection

Data were collected from previous work, at different period of time result were checked by experimentally using microprocessor controlled 23-L fermenter.

Boundary conditions

The point which satisfies the model equation, the boundary condition that are taken for validation of the model are given below

X = 0 g/l

S= S_o g/l,

T = 0 hr and Ethanol = 0 g/l

Previous model

Previous model is taken from previous research, equation I, II, III were selected as a cell growth, ethanol production and substrate utilization model for ethanol production from molasses using the rmotolerant *klyueromyces marxianus*.

$$\frac{dx}{dt} = \mu_{max}\left(\frac{S}{k_{xx}+S}\right)x \qquad (I)$$

$$\frac{dP}{dt} = q_{\max}\left(\frac{S}{k_{sp}+S}\right)x \qquad (II)$$

$$\frac{dS}{dt} = -\left(\frac{1}{Y_{\frac{x}{s}}}\frac{dx}{dt}\right) - \left(\frac{1}{Y_{\frac{p}{s}}}\frac{dP}{dt}\right) \qquad (III)$$

Where μ_{max} = maximum cell growth, X=cell growth, S = substrate utilization, kxx = half saturation constant, $q_{\max}$ =maximum specific growth,Yx/s = yeild coefficient cell growth with respect to substrate utilization Yp/s = yield coefficent ethanol production with respect to substrate utilization.

Validate model

Above equations I, II and III were validate using experimental data by ode 45 packages in Mat lab software. The equation was validate using different factor by taking “a” as a maintenance which is 0.3 and 0.9 correction factor equation IV,V,VI are the validate equation according to experimental work.

$$\frac{dx}{dt} = \mu\left(\frac{s}{k_{xx}+s^a}\right)\sqrt{x} \qquad (IV)$$

$$\frac{dP}{dt} = Y_{\frac{p}{x}}\mu\left(\frac{s^a}{k_{\frac{s}{p}}+s}\right)x^{0.9} \qquad (V)$$

$$\frac{dS}{dt} = -\left(\frac{1}{Y_{\frac{x}{s}}}\frac{dx}{dt}\right) - \left(\frac{1}{Y_{\frac{p}{s}}}\frac{dP}{dt}\right) \qquad (VI)$$

Where X=cell growth, S=substrate utilization, kxx =half saturation constant, Yx/s=yeild coefficient cell growth with respect to substrate utilization Yp/s = yield coefficent ethanol production with respect to substrate utilization.

RESULTS AND DISCUSSION

Monod model that was used to validate, three equations were validate such equation relate to the cell growth, substarate and ethanol production.

Cell growth model

During a process of fermentation, yeast is used to convert molasses into ethanol. Cell growth is one of the important steps in ther process of fermentation; the data were selected from previous study to validate the model (Fig.2-11) for further study. The model is validated using *kluyeromyces marxianus* (Fig. 2-5). Model results show the approximately same results as for experimental results were concerned. Cell growth increases as time increases .in above graph, equation also given for cell growth, in this equation powered “a” is for correction factor. Because when we discuss some process, there is need to see which factor affect.

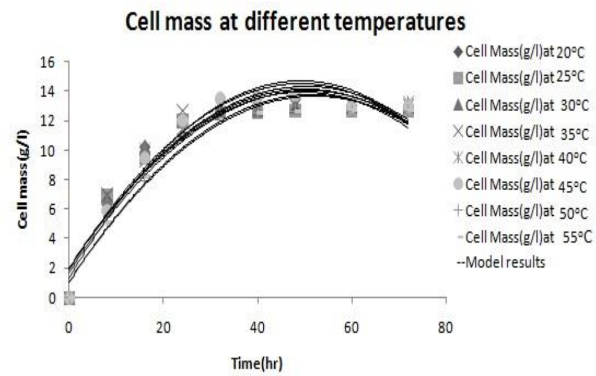


Fig. 2: Cell mass at different temperatures for keeping other variable of optimized conditions

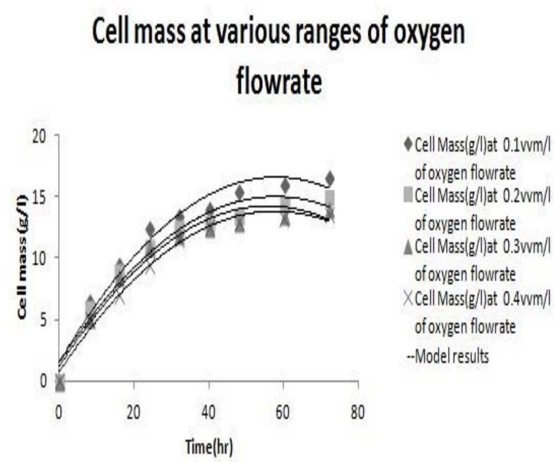


Fig. 3: Cell mass at different Oxygen flow rate for keeping other variable of optimized conditions

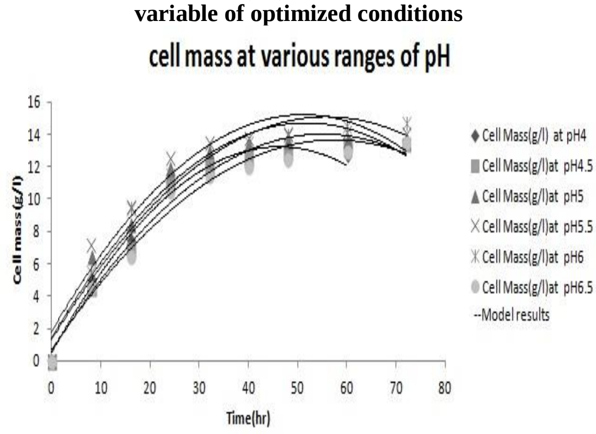


Fig.4: Cell mass at different pH for keeping other variable of optimized conditions

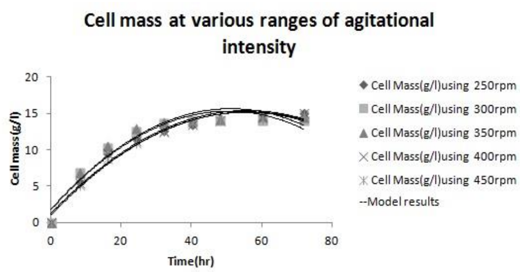


Fig. 5: Cell mass at different Agitation intensity for keeping other variable of optimized conditions Substrate utilization model

During a process of fermentation, substrate utilized for the growth of microbes and make conditions for ethanol production, in this we validate the previous model for substrate utilization (Fig. 6-9). From previous models some constant of verifications were made to optimize the various parameters for ethanol production. During conversion of substrate into products some process parameter involved to optimize this parameter there is an increment of constant terms for indicating verification in fermenter.

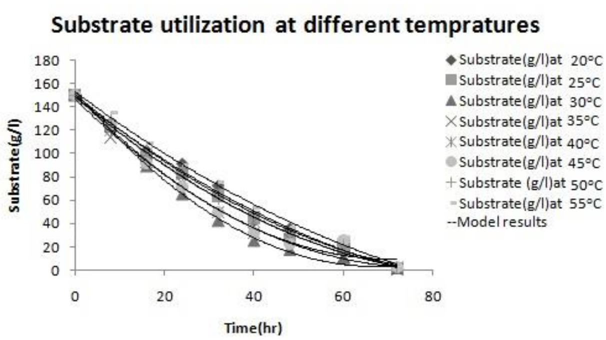
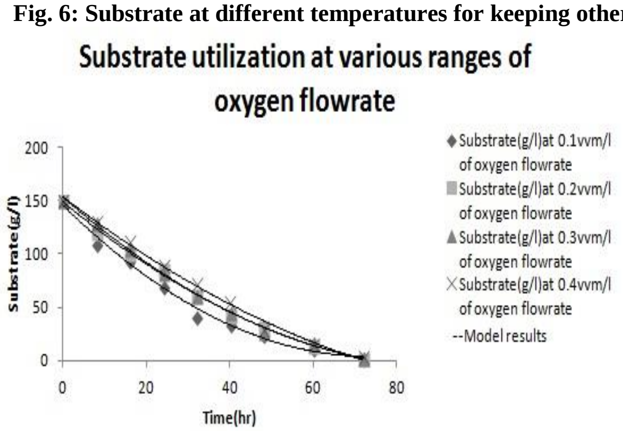


Fig. 6: Substrate at different temperatures for keeping other



variable of optimized conditions

Fig. 7: Substrate at different Oxygen flow rate for keeping other variable of optimized conditions

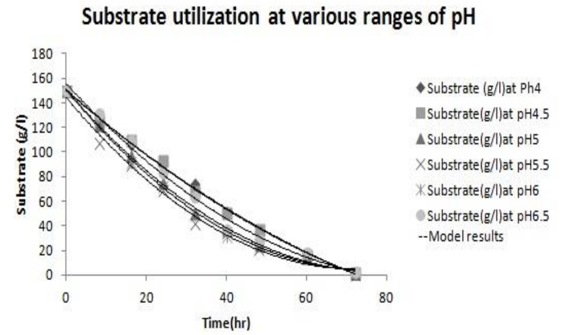


Fig. 8: Substrate at different pH for keeping other variable of optimized conditions

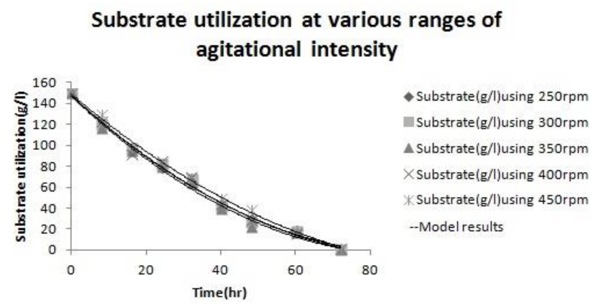


Fig. 9: Substrate at different Agitation intensity for keeping other variable of optimized conditions

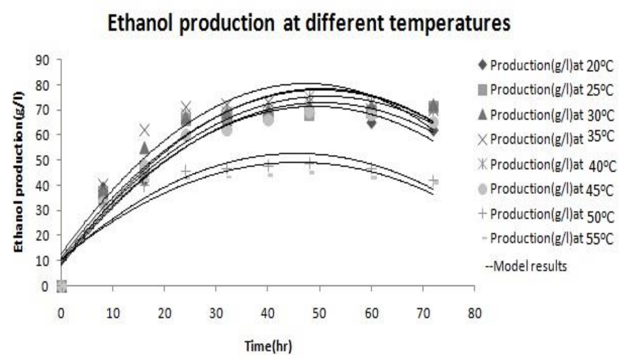


Fig. 10: Production at different temperatures for keeping other variable of optimized conditions

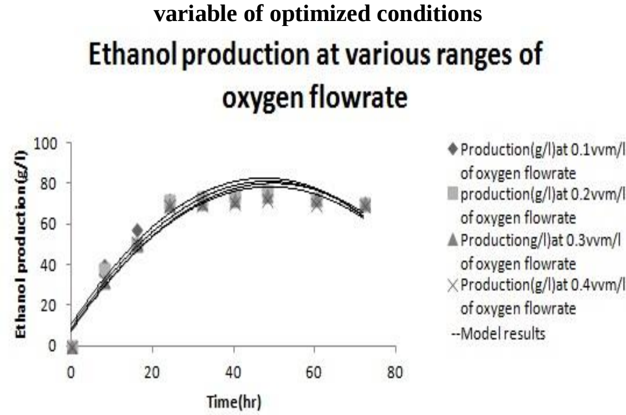


Fig. 11: Production at different oxygen flow rate for keeping other variable of optimized conditions

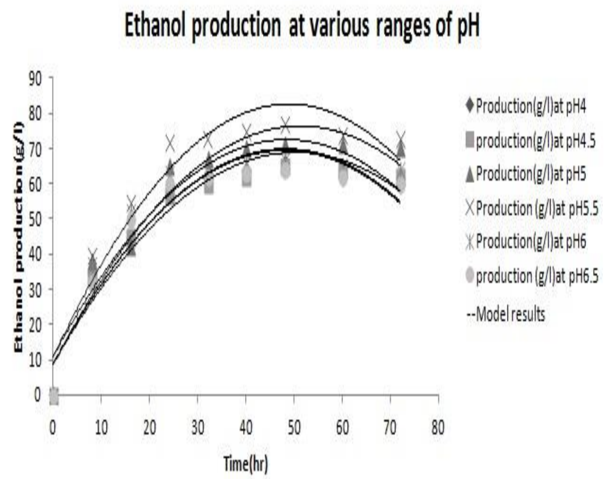


Fig. 12: Production at different for keeping other variable of optimized conditions

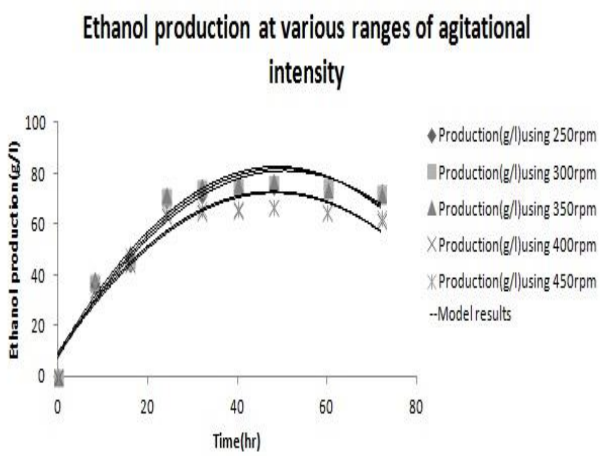


Fig. 13: Production at different Agitation intensity for keeping other variable of optimized conditions

Production model

From these models, some constants were adopted due to the utilization *kluyeromyces marxionus* and the correction factor like inhibition factor during conversion of substrate into the final product. There is, however, a need to identify some factor that will affect production of ethanol from molasses. Different carbon and nitrogen source were used to see the effects of various parameters and finally models were developed for production of ethanol (Fig. 10-13).

CONCLUSION

Mathematical modeling can be used to optimize various parameters without using any experimental setup: Time saving for the laborious work by using a mathematical model, we can predict the next calculation. Money saving for purchasing large machineries. No laboratory experiment is needed after developing a mathematical model to optimize kinetic parameters.

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