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Mathematical Modeling of Ethanol Production through Batch Fermentation of Glucose with Kluveromyces Marxianus

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ABSTRACT

Mathematical models are a means of representing essential aspects of reality (process, phenomenon, object, element, system, etc.) with the help of mathematical constructs. 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. This research developed a mathematical model that illustrated the kinetics of ethanol production, incorporating both fermentation time and temperature from the batch fermentation of glucose with Kluveromyces Maxianus. Glucose biomass was found to decrease linearly with temperature rise and the modified Gompertz model was used to describe the ethanol production. The arhenious plot was used to illustrate the temperature dependence rate of the reaction. Matlab 9.0 and Microsoft Excel 2007 were the statistical software used for the iteration and the estimation of the biological parameters. The derived mathematical model could be adapted to illustrate the kinetics of ethanol production to the stationary phase during the fermentation of glucose as influenced by temperature and fermentation time using Kluveromyces Maxianus.

Keywords: Modeling, Temperature, Energy, Fermentation time, Ethanol, Biomass, Glucose, Kinetic, Kluveromyces marxianus.

1.0 INTRODUCTION

Over the last century, energy consumption has increased steadily as the world population has grown and more countries have become industrialized. Crude oil has been the major resource to meet the increased energy demand (Balat and Cahide, 2008). Considering the economy in this nation and many other nations that depends on oil, the consequences of inadequate oil availability could be severe. Therefore, there is a great interest in exploring alternative energy sources (Mariono and Grossmann, 2011).

In view of these, finding an alternative renewable energy source that is both economical and environmentally friendly is of great interest to researchers (Watt *et al*., 2007 Ye Sun, 2002). A major proposed alternative is ethanol. Ethanol can be used in mixture with fuels for gasoline engines; it has higher octane index and higher heat of vapourization than gasoline (Lopez, 2010). Also, (Mariono and Grossmann, 2010), confirmed ethanol as an alternative fuel that can be implemented in the short term for the transportation sector owing to its compatibility with automobile engines, and it takes advantage of existing supply chain of liquid fuels that is already well established and thus it production has been supported by government policies and stakeholders.

With the growing interest of researchers and great economic potential ethanol has, as an alternative to fossil fuels, fermentation technology must care for several variables involved in the production of ethanol to optimize its production process (Manikandan and Viruthagiri, 2011; Neelakandan and Usharani, 2009). A major operating variable is temperature (Gorsek and Zajsek, 2010[a]; Jesper, 2005). Therefore, for optimum output of ethanol concentration, the influence of temperature should be investigated.

In the last decades, continuing progress has been observed in applications of mathematical models in biological growth (Gorsek and Zajsek, 2010[b]). This research develops a mathematical model of the kinetics of ethanol production as influenced by temperature variation and fermentation time using the experimental result of the batch fermentation kinetics of a novel thermotolerant strain of the yeast *Kluveromyces Marxianus* by Hughes, *et al.*, (1984).

2.0 MATERIAL AND METHODS

2.1 Experimental Data.

The experimental data utilized by this study was the batch fermentation kinetics of a novel thermotolerant strain of the yeast *Kluveromyces Marxianus* evaluated between 30°C and 48°C by (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 Models Parameters

These are parameters that are involved in the growth of cell during fermentation process.

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 and,

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

E_P = activation energy for ethanol production (KJ/kmol)

θ = temperature (^{0}C)

t = fermentation time (h)

There are standard biological models that can be used to describe biochemical processes successfully (Nduke, 2009; Zwietering *et al.*, 1990). The experimental data were subjected to different kinetics models and the model that best fit the experimental data was adopted.

2.3 Modeling Change in Biomass with Temperature

From the experimental data, the rate of change of glucose biomass, i.e. biomass increase with temperature is discovered throughout the fermentation process to be negative. The experimental data is fitted into Microsoft excel 2007 to get the relationship between temperature and biomass, the relationship is illustrated by eq (1) below.

$$X = k_1 - k_2\theta \quad \text{...(1)}$$

Where θ is the temperature (^{0}C), X is the biomass after 24h fermentation time (g/l), where $k_1 and\ k_2$ are constants which represent glucose biomass decrease with temperature (g/l ^{0}C). Using Microsoft excel curve fitting method, the values of $k_1 and\ k_2$ estimated from the experimental data in the range of (30 – 48) ^{0}C were obtained.

2.4 Modeling Ethanol Mass Concentration

Experimental data available revealed that the mass concentration of ethanol was affected by temperature over the fermentation period. Modified Gompertz model could be regarded as adequate in describing the behavior of the ethanol mass concentration with temperature by thermotolerant strain of *Kluveromyces Maxianus* over the fermentation period.

The Gompertz's law of mortality is commonly known as the most successful law to model the dying out process of living organisms. It is represented by:

$$S(x) = g^{c^x} \quad \text{...(2.1)}$$

Where *x* is the age and *c* and *g* are constants. S(x) predicts the number of survivors of age *x*. Gompertz used the double exponential function in the formula to explain the increased inability to withstand destruction (Willemse and Koppelaar, 2000). The model was later expanded to a function that could describe organ cell growth (Okpokwasili and Nweke, 2005):

$$y = a.\exp[-\exp(b - ct)] \quad \text{... (2.2).}$$

Where y = concentration

a = potential maximum concentration

t = time

b and *c* are constant

The modified Gompertz model was obtained by the following mathematical modifications.

To obtain the inflection point of the curve, the second derivative of the function with respect to *t* is calculated:

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$$\frac{dy}{dx} = ac.\exp[(b-ct)].\exp(b-ct) \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots (2.3)$$

$$\frac{d^2y}{d^2x} = ac^2\exp[-\exp(b-ct)].\exp(b-ct).[\exp(b-ct)-1] \dots\dots (2.4)$$

At the inflection point, where $t = t_i$, the second derivative is equal to zero:

$$\frac{d^2y}{d^2x} = 0 \rightarrow t_i = \frac{b}{a} \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots (2.5)$$

The expression for maximum growth rate can be derived by calculating the first derivative at the point of inflection.

$$\mu_m = \left(\frac{dy}{dx}\right)_{t_i} = \frac{ac}{e} \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots (2.6)$$

The parameters c in the Gompertz equation can be substituted for by

$$c = \frac{\mu_m e}{a}$$

The description of the tangent line through the inflection point is:

$$y = \mu_m.t + \frac{a}{e} - \mu_m.t_i \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots (2.7)$$

The lag time is defined as the t-axis intercept of the tangent through the inflection point:

$$0 = \mu_m.\lambda\frac{a}{e} - \mu_m.t_i \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots (2.8)$$

Combining equation 2.5, 2.6 and 2.8 gives:

$$\lambda = \frac{(b-1)}{c} \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots (2.9)$$

The parameter b in the Gompertz equation can be substituted by:

$$b = \frac{\mu_m e}{a}\lambda + 1 \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots (2.10)$$

The asymptotic value is reached for t approaching infinity:

$t \rightarrow \infty: y \rightarrow a \qquad A \Rightarrow a$

The parameter a in the Gompertz equation can be substituted for by A, this is thus the modified Gompertz Equation.

$$y = Aexp\left\{-exp\left[\frac{\mu_m \exp(1)}{A}(\lambda - t) + 1\right]\right\} \dots\dots\dots (2.11)$$

Where μ_m maximum specific growth rate (h^{-1})

$$\mu_m = Pr_m,$$
$$A = A_m$$
$$y = A_{Etoh}$$

This gives:

$$A_{EtoH} = A_m\, exp\left\{-exp\left[\frac{Pr_m \exp(1)}{A_m}(\lambda - t) + 1\right]\right\} \dots\dots (2.12)$$

The kinetic parameters are:

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 and,

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

According to the experimental data, it is obvious that all the parameters of the experiment are affected by temperature.

We therefore expressed the maximum ethanol production rate P_{mr}, the time lag λ, and the maximum ethanol mass concentration A_m as functions temperature.

The maximum ethanol production rate was expressed as a linear function of temperature:

$$P_{mr} = a\theta + b \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots (2.13);$$

The time lag t_l, was expressed as an exponential function of temperature:

$$\lambda = c.exp^{d\theta} \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots (2.14)\ ; \text{and}$$

the maximum ethanol mass concentration was expressed as a polynomial of temperature:

$$= A_m = e\theta^2 + f\theta + g \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots (2.15)$$

Where a, b, c, d, e, f, and g are constants

Thus, equation 2.15 becomes

$$A_{EtoH} = (e\theta^2 + f\theta + g)exp\left\{-exp\left[\frac{(a\theta + b)\exp(1)}{(e\theta^2 + f\theta + g)}\left(\left(c.exp^{d\theta}\right) - t\right) + 1\right]\right\} \ldots\ldots (2.16)$$

2.5 Temperature Dependent Maximum Ethanol Production Rate

The Arrhenius equation is a simple and remarkably accurate formula to illustrate the dependence of the temperature on reaction rate constant, and rate of a chemical reaction (Levine, 2005). The theory of the temperature effect on the reaction rate originated from the temperature effect on the equilibrium constant. It is known that:

$$\frac{dLnK}{d\frac{1}{T}} = -\frac{H}{R} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (2.17)$$

Where,

K = equilibrium constant,

R = the gas constant and,

H = the heat of reaction.

Where E referred by Arrhenious as representing the energy difference between the reactants and an activated species. The term E is therefore called Activation Energy. Taking E as a constant equation 2.17 can be integrated to yield:

$$Ln\ k = Ln\ A - \frac{E}{RT} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (2.18)$$

Where Ln A is the constant of integration. Equation 2.18 can be converted to:

$$k = Ae^{-\frac{E}{RT}} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (2.19)$$

The temperature dependent ethanol rate can clearly be expressed by this Arrhenious relationship.

$$P_m = P_{mo}\, e^{-\frac{E_p}{RT}} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (2.20)$$

where P_m is the maximum ethanol production rate (g/Lh), E_p represents the activation energy of ethanol production (KJ/mol), T is the temperature in Kelvin, R is ideal gas constant (8.314KJ/mol K) and P_{mo} is the pre – exponential factor (g/Lh).

3.0 RESULTS AND DISCUSSION

3.1 Effect of Temperature on Biomass

The batch fermentation kinetics of a novel thermotolerant strain of the yeast *Kluveromyces marxianus* were evaluated between 30°C and 48°C by (Hughes, *et al* 1984). In their study, the kinetics of ethanol formation from glucose in batch culture by thermotolerant *Kluveromyces marxianus* was reported over the same temperature range (30°C - 48°C). Figure 3.1 shows the glucose biomass decrease with temperature rise.

Figure 3.2 shows the influence of temperature of glucose biomass decrease with temperature by thermotolerant strain of *kluveromyces Maxianus.* The figure shows both experimental and modeled equation. The linear equation was found to be the appropriate with (R^2 = 0.97) to successfully describe the temperature dependence of biomass decrease fermentation with the range of 30 – 48^{0}C, and the estimated values of $k_1 and\ k_2$ were (20.74 and 0.391) respectively.

Temperature had a moderate negative linear impact on the glucose biomass increase by thermotolerant strain of *kluveromyces Maxianus.* Thus the equation (2.1) successfully describe the relations between the biomass decrease and temperature.

3.2 Results of Gompertz Model

The Modified Gompertz model adopted for this study incorporate about seven constants which were used to express the maximum ethanol production rate (P_{mr}) the time lag (λ), and the maximum ethanol mass concentration (A_m) as functions temperature.

The constants *a, b, c, d, e, f, and g* were evaluated by Microsoft Excel, 2007 and the predicted values are shown in the tables 3.1, 3.2 and 3.3.

Figure 3.3, 3.4, 3.5, 3.6 and 3.7 show the result of the experimental data and Gompertz model in demonstrating the temperature variation of ethanol production from the thermotolearant strain of *Kluveromyces Maxianus* of glucose. . 48^{0}C and 45^{0}C have the same determination coefficient value with R^2 = 0.97 followed by 30^{0}C with R^2 of 0.95, while 43^{0}C has the lowest value with an R^2

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of 0.86 and the highest is at 40^0C with $R^2 = 0.98$. The average determination coefficient R- Square was 0.928. This determination coefficient however shows that the model can describe the fermentation process of ethanol production by this strain of yeast.

3.3 Maximum Ethanol Production Rate

The maximum ethanol production rate was illustrated by arrhenious plot shown in figure 3.8. The maximum value of P_{mr} was found at 43^0C which agrees with the experimental data. The activation energy for this yeast was estimated to be 80KJ, From equation 3.2, *Ln k* represents the logarithm of $P_{mr,}$ which is plotted against T^{-1}, *Ln A* represent the logarithm of P_{mo}. The temperature dependency of the maximum ethanol production rate was fitted very well the experimental data.

The Activation Energies of emzymes reaction ranges between E_p = (40 – 80)KJ/mol according to (Gorsek and Zajsek, 2010[a]). The value of the activation energy E_p of ethanol production by this strain of *Kluveromyces Maxianus* was estimated to be approximately 80KJ/mol which falls between the values stated in the literature.

4.0 CONCLUSION

From the results of both the experimental and mathematical models, it could be revealed that the results show little difference. It can therefore be said that the use of mathematical model will contribute to a better understanding of effects of various factors affecting the production of ethanol. This means it will enable us to design and control the fermentation process to deliver an optimised output and also serve as means for process improvement.

The use of mathematical models had contributed and will still continue to contribute to a better understanding of the environmental effect of the biomass activities and the production of bio – products. Insight gain could be used to as tools to further enhance the productivity of biological and bio-chemical processes.

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The effort of Hughes et al., 1984 is greatly acknowledged in providing the experimental data that serves as the basis for this research work.

TABLES

Table 3.1: Estimated value of *a and b*

Constants	*a(g/L^{0}C)*	*b(g/L)*	*R^2*
Values	0.145	-2.46	0.859

Table 3.2: Estimated value of c *and d*

Constants	*c(h/^{0}C)*	*d(^{0}C)*	*R^2*
Values	0.112	0.094	0.983

Table 3.3: Estimated value of *e, f and g.*

Constants	*e(G/L$^0C^2$)*	*f(G/L^{0}C)*	*g(g/l)*	*R^2*
Values	-0.287	20.4	-283.3	0.977

FIGURES

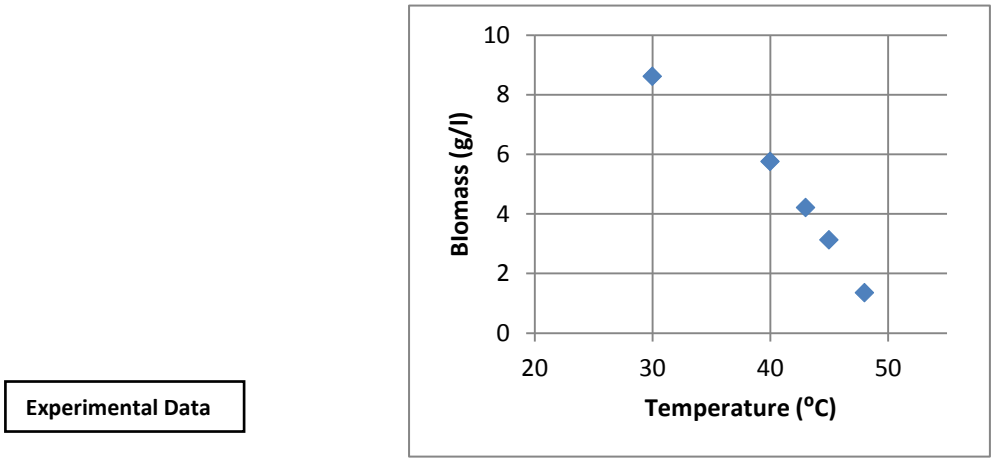

Figure 3.1: Biomass negative increase with temperature

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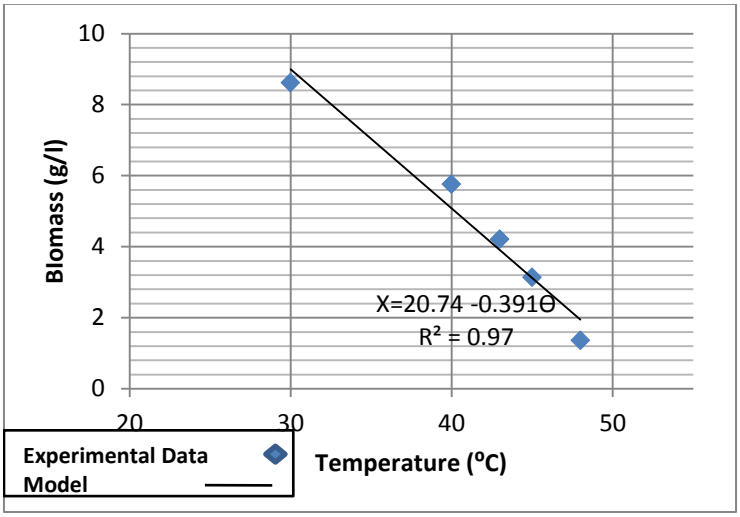

Figure 3.2: Influence of Temperature on Glucose Biomass Decrease

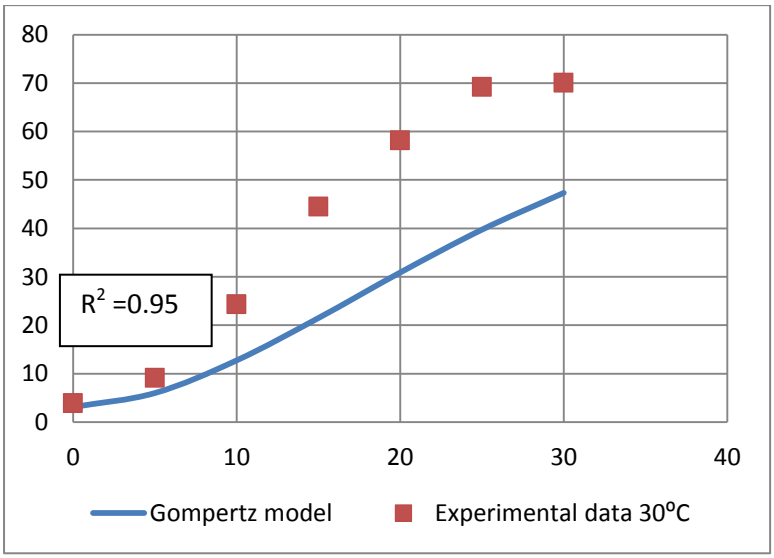

Figure 3.3 Influence of Temperature on ethanol yield at 30^0C

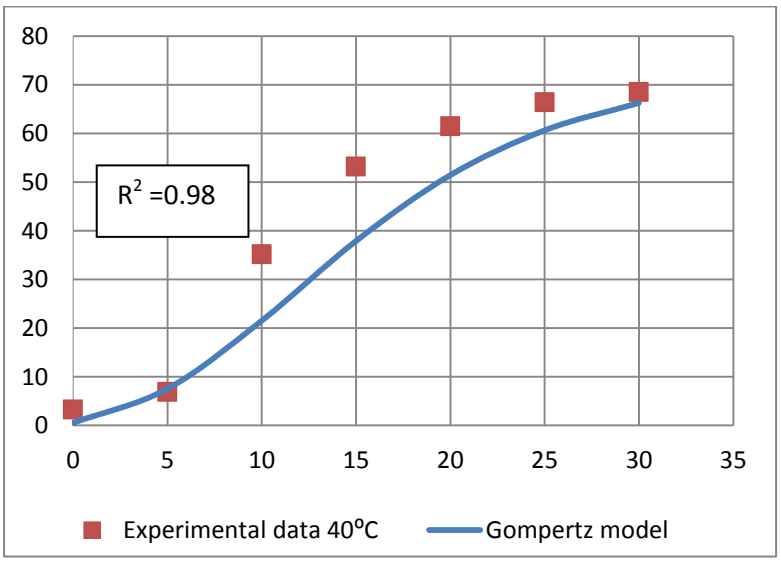

Figure 3.4 Influence of Temperature on ethanol yield at 40^0C

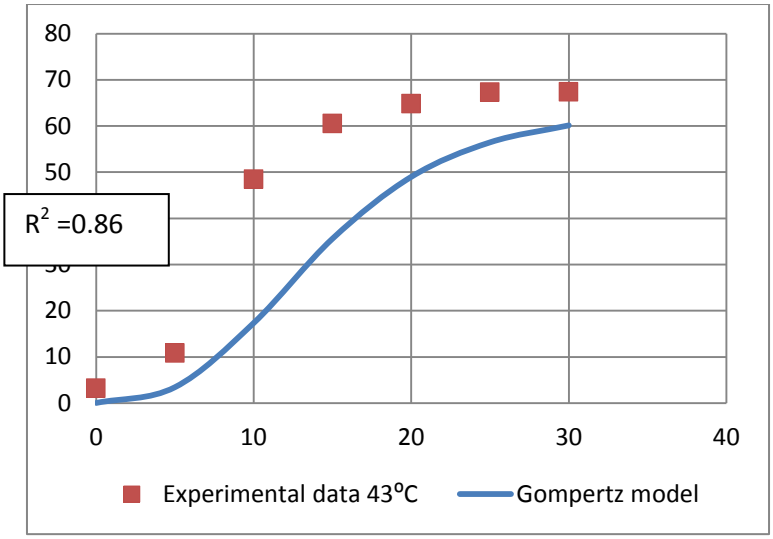

Figure 3.5 Influence of Temperature on ethanol yield at 43^{0}C

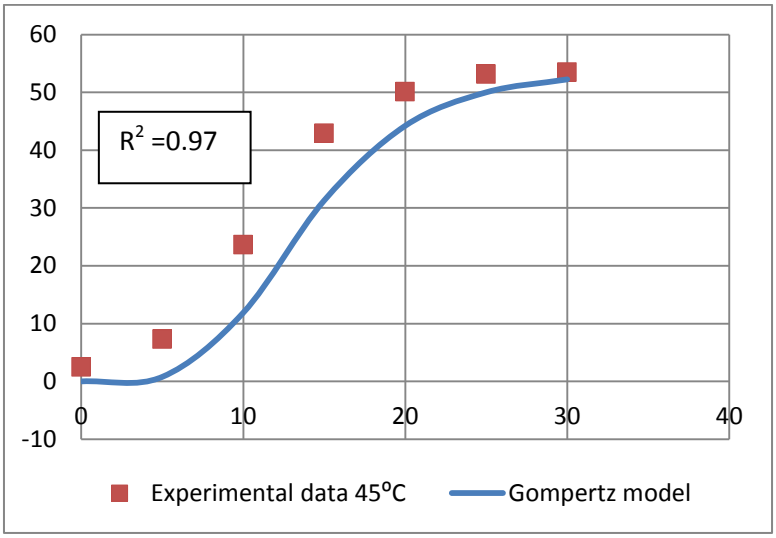

Fig 3.6 Influence of Temperature on ethanol yield at 45^{0}C

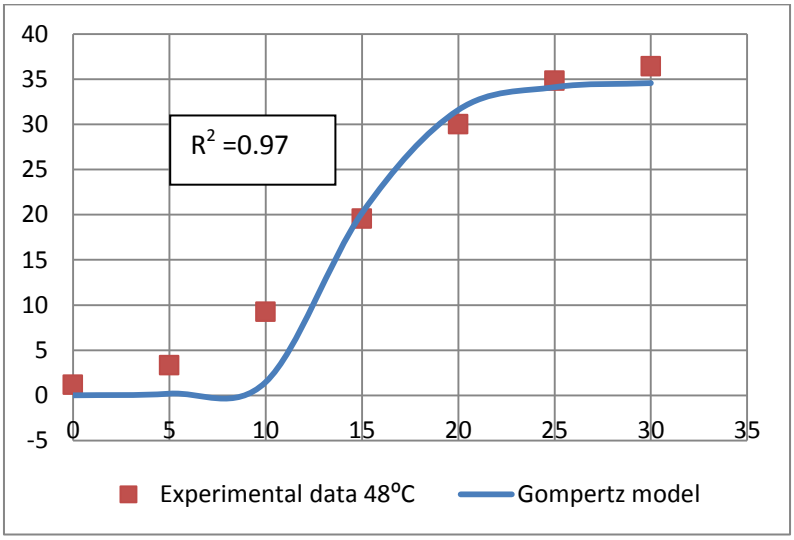

Fig 3.7 Influence of Temperature on ethanol yield at 48^{0}C

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Ln **Pmr = 17.89-5.24 Ep/TR**

R^2 = 0.894

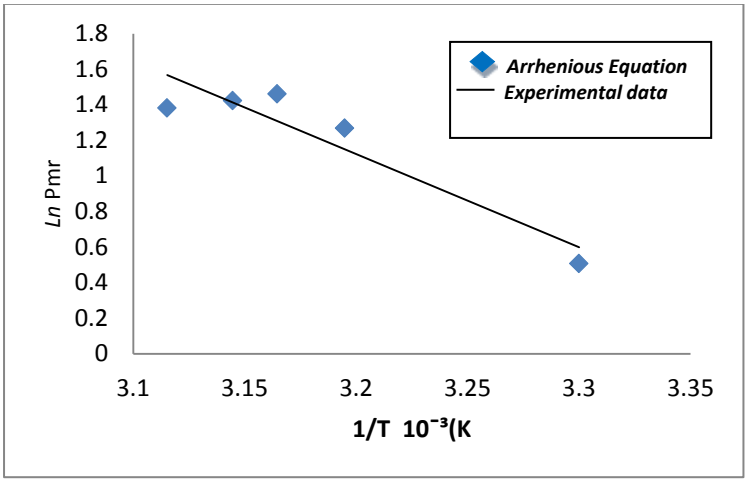

Fig 3.8 Arrhenious plot for Ethanol Production by *Kluveromyces Maxianus*