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Prediction and Analysis of Variable Parameters of some established models in Batch Beer Fermentation

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Abstract:In this work, established models of renowned scholars in fermentation technology are analytically solved. Fermentation experiments were also performed on the production of ethanol and biomass from substrate (grain i.e. malted barley) with time and used to validate the analytical solutions of the scholarly models. The result shows that the models were real and true to life as they gave coefficient of correlation of 99.63%. It is also observed that during this fermentation, there was serious interaction between substrate concentration and ethanol concentration, substrate concentration and biomass concentration. From this model, it was found that the yield of ethanol (product) was 79.34%, yield of biomass was 43.8%, initial ethanol before fermentation was 1.45g/lit. Substrate at the beginning, S_0= 8.114g/lit. and initial biomass X_0 was 0.8098g/lit. This result can be applied in fermentation planning in any brewing company of research centers to predict variation of certain parameters.

Keywords: Models, batch beer fermentation, growth, biomass, yeast, alcohol.

Introduction

Background of study

The term "fermentation" can be used in its original strict meaning (to produce alcohol from sugar) or it can be defined as the microbial action controlled by man to make useful product from sugar. Among the products of fermentation, ethanol is the most popular and widely used. This is because it has remarkable characteristics which distinguish it as the best alternative fuel for automobiles. It is obtained from anaerobic degradation of starchy or cellulosic material by microbes such as yeast, bacteria, mould etc. [2]

Simple sugars are crystalline, soluble in water and have a sweet taste. It is a form of carbohydrate. It can be subdivided into two:

1. Monosaccharide; example - glucose, fructose, gelatos. They have one molecule and their molecular formula is $C_6H_{12}O_6$.[1]
2. Disaccharides; example - sucrose (glucose + fructose), lactose (glucose + gelatos) and maltose (glucose + glucose). They are constituent of cellulosic waste, example, sawdust or starch.

It is a product of the hydrolysis of cellulose using an enzyme called cellulax. When fermented by brewer's yeast gives ethanol and CO_2. The most common example of simple sugar is the monohydric which include glucose and fructose.

Yeast are classified as micro organisms from the fungi family called ascomycetes (which have sac-like structure). They are reproduced by budding, fission and sporulation, they are about 20µm and 7µm in length and diameter respectively. Yeast are available is a wide range and they contribute greatly in the creation of various alcohols ranging from mild ones such as beers to the medium such as wines to strong ones such as Vodka. Types of yeast used affect the rate of production or fermentation of the sugar; this is because different yeasts have different temperature ranges that they can withstand during fermentation. About 30 species of Saccharomyces have been distinguished but the commonest ones are Saccharomyces cerevisae (top fermentation or ale fermentation) and Saccharomyces carlsbergeniss (bottom fermentation or lager yeast). The problem with yeast is that it is limited by alcohol tolerance, the alcohol ends up killing the yeast. [6][9]

Table 1.Yeast strains and their relative fermentation efficiency [14]

Yeast strains	Ethanol per ton of molasses(gallons)	Efficiency (%)
ATCC 4132	93	73
CBS 1237	90	70
Y 7494	86	67
UCD 505	83	65
UCD 595	81	63

ATCC 26603	81	63
DADY	77	60
BAKER	77	60
NCYC 90	57	44

Source of Yeast

ATCC:	American type culture collection
CBS:	Center Albureanu Voor Schimenlcatues, the motherland
UCD:	University of California Davis
DADY:	University Foods Corporation
BAKER:	Local Procurement
Y:	Northern Region Research center, USA.

Yeast life cycle

The life cycle of yeast counts from when it is inoculated into the medium. It follows four phases, [3] in which all of the phases may overlap in time.

Lag phase

This is the phase in which the yeast stores up glycogen in its cells and uses it as a source of energy and for production, since the sugars are not assimilated. This phase is marked by a drop in pH, because of utilization of phosphate and a reduction in oxygen [12].

Growth Phase

This is referred to as the respiration stage. It follows the lag phase once sufficient reserves are built up within the yeast. The covering of foam on the wort surface due to liberation of CO_2 shows that growth has occurred. In this stage, the yeast cells use up the oxygen in the wort to oxidize a variety of acid compounds resulting in a significant drop in pH [10].

Fermentation phase

This follows immediately after the growth stage when the oxygen supply has been reduced. It is an anaerobic process. This stage involves reduction in sugar medium and production of CO_2, ethanol and other by-products. At this stage, yeast is mostly in suspension, allowing itself disperse at maximum contact with the medium to quickly convert fermentation sugar [5] [4].

$$CO_2 + C_2H_5OH + \text{by-product} \xleftarrow{\text{Anaerobic}} \text{Sugar}$$

Flocculation Phase

This is also known as sedimentation phase. It is the process through which yeast flocculates and settles to the bottom or top of the vessel. Most yeast flocculates after three to seven days. The yeast produces a substance called glycogen when it undergoes a process of preserving its life [11].

Physical Properties of Ethanol

1. Ethyl alcohol is a clear colourless liquid.
2. Has a characteristic taste and smell.
3. It has no effect on litmus paper.
4. It is very soluble in water due to the presence of hydroxyl group.
5. It has a boiling point of 78°C and a freezing point of -117.8°C.
6. It gives a burning sensation in the mouth when swallowed. That is why it is called burning water i.e. “aqua ardens”.
7. It has a density of 789kg/m^3 and a refractive index of 1.36.
8. It forms an azeotropic mixture on boiling [13]

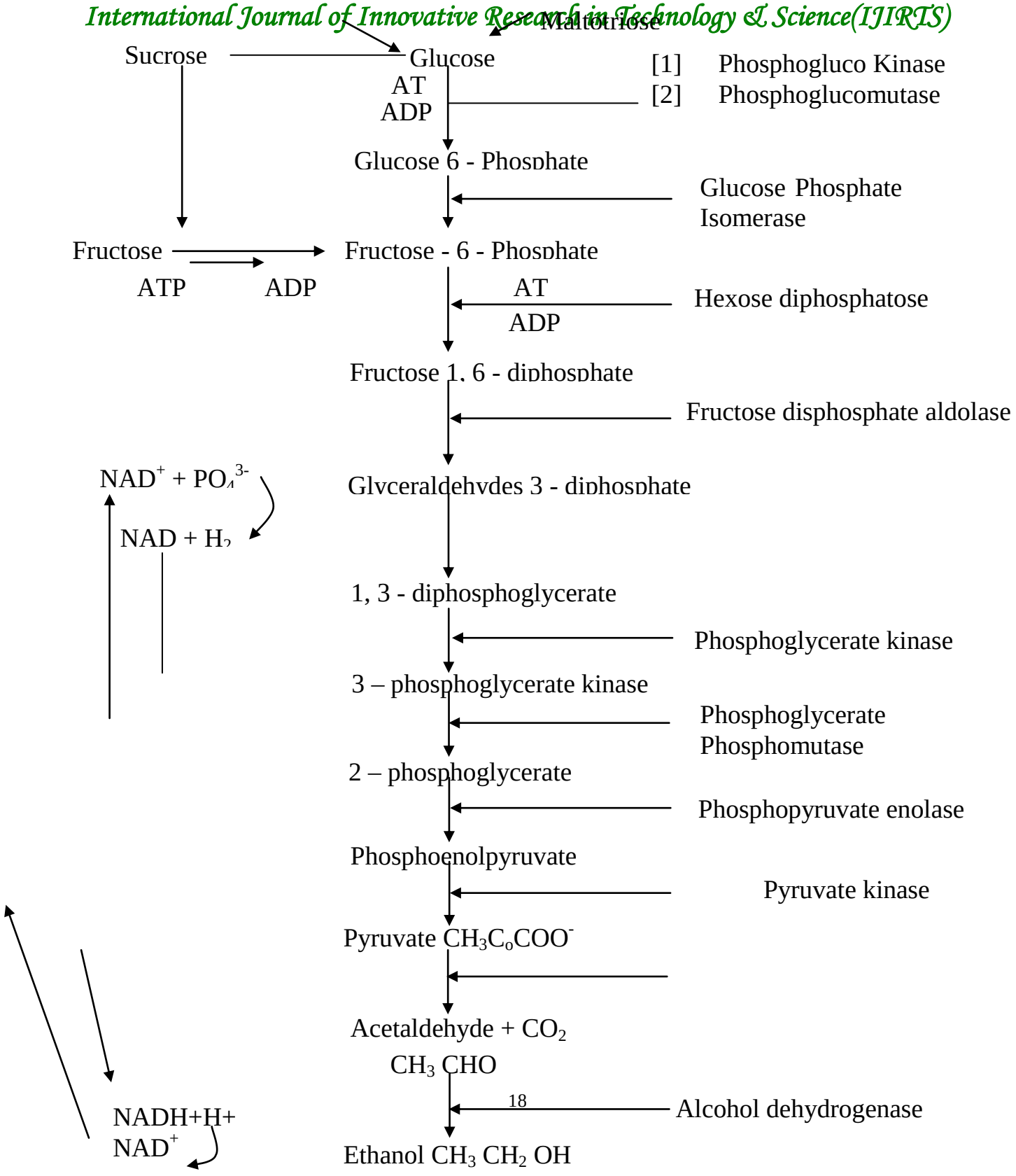

Figure 1. Yeast life cycle

The problem is that amongst the numerous models formulated by different authors, there has not been proper and extensive analysis and predictions of those models made. In most cases, the models are not even solvable analytically but computer-wise and hence lack of full or complete analysis of what obtains in the mechanism of the fermentation process.
It is important and significant to study, in details, the full and intricate mechanism of what obtains during the kinetics of fermentation of beer. This will help the brewers to know where to add or subtract additive in other to have optimum beer production.
The objective or aim of this study is to solve analytically some of the established models of different authors for beer fermentation and use experimental values to validate them and their parameters so as to see how well the models fit. Models untested and unsolved are just mathematical finery that may or may not fit the empirical values. If they fit well, then predictions can be made with them, otherwise, they will be jettisoned. This will help the brewer of beer know more about the most accurate and complete fermentation stages and of course enhance in a good brew.
This work will cover trying to offer analytical solutions to some established models. It does not include establishing more models or expanding the mechanism of fermentation of beer
.

Review of Model development

Many models have been developed on beer fermentation with a view to touch different aspects of their kinetics. [7] postulated that the new beer fermentation model can be developed based on fundamental knowledge of biochemical pathways.
This model can be subdivided into growth model, amino acid model and aroma and flavour model.

A Flavour Model for Beer Fermentation

Under biomass.product $\frac{dx}{dt} = \mu x$, so that $x = x_0 e^{\mu t}$ (1)
Under growth model, we have sugar consumption as
Glucose $\frac{d_G}{dt} = -\mu_1$
With a solution of $G = G_o + {}^{\mu_1}/_{\mu} X_0(1 - e^{\mu t})$ (2)
Maltose; $\frac{dM}{dt} = -\mu_2 X$ so that $M = M_0 + \frac{\mu_2}{\mu} X_0(1 - e^{\mu t})$ (3)
Maltotrioses; $\frac{dN}{dt} = -\mu_3 X$
With the solution as $N = N_0 + \frac{\mu_3}{\mu} X_0(1 - e^{\mu t})$ (4)
Also, under ethanol production
$E = E_0 + Y_{EG}(G_0 - G) + Y_{EM}(M_0 - M) + Y_{EN}(N_0 - N)$
With a solution as
$E = E_0 - (Y_{EG}\mu_1 + Y_{EM}\mu_2 + Y_{EN}\mu_3)\mu X_0(1 - e^{\mu t})$ (5)
Under liquid phase carbondioxide production

$$\frac{dC}{dt} = K_C(C_S - C)$$

With solution as
$C = C_S - (C_S - C_0)e^{-kt}$ ---------- (6)

Alcohol Fermentation in Brew with Immobilized Cells

[16] and [15] writing under the title "modeling of alcohol fermentation in brewing, comparative assessment of flavour profile of beers produced with free and immobilized cells" posited that fermentation with immobilized cells can be described by the following equations:
For biomass $\frac{dx}{dt} = \mu_t X_t$
With solution as $X = X_0 e^{\mu t}$ (7)
For the production of alcohol $\frac{dp}{dt} = q_t X_t$
With the solution as $P = P_0 - \frac{qx_0}{\mu} - (1 - e^{\mu t})$ (8)
And the remaining substrates
$\frac{ds}{dt} = -\frac{1}{Y_{X/S}} \cdot \frac{dx}{dt} - \frac{1}{Y_{P/S}} \cdot \frac{dp}{dt}$
Multiplying through by dt and integrating yields a tripartite or 3-dimension consideration of biomass, product and substrates solution as
$S = S_0 - \frac{1}{Y_{X/S}}(X - X_0) - \frac{1}{Y_{P/S}}(P - P_0)$ (9)

Data Collection

Part of the data for validation of the above models was collected from Awonmama Brewing Company and part was obtained from other researchers' experimental data.

Curve Fitting

A MATLAB package 7.9 was used to fit the experimental values to the models. Scatlar diagrams of experimental data were plotted and the analytical solution models of each scholar were superimposed on the scatlar-diagram to check for the goodness of fit and validity of the model theory.

3.5 Algorithm for making 3-D surface response plot.

1. Write out the values of X_1, X_2 and Y.
   X_1 = [ ];
   X_2 = [ ];
   Y = [ ];

2. Go statistical; regstats (y, [x_1,x_2], "quadratic")
   This regstats command truncates the cubic models in the MATLAB toolbox at the term containing a_5 that is;
   $Y = a_0 + a_1X_1 + a_2X_2 + a_3X_1X_2 + a_4X_1^2 + a_5X_2^2$

3. As beta values are entered, the toolbox declares a_i values.
   a_0 =; a_1 =; a_2 =; a_3 =; a_4 =; a_5 =;

4. Write mesh command
   [X_1 X_2] = mesh grid ($X_{1(min)}$: X_1: $X_{1(max)}$, $X_{2(min)}$: X_2: $X_{2(max)}$);

5. Write out the truncated quadratic model with its declared a_i's
   $Y = a_0 + a_1*X_1 + a_2*X_2 + a_3*X_1*X_2 + a_4*X_1\text{^}2 + a_5*X_2\text{^}2$

6. Write out the surface plot and enter
   Surfc (X_1, X_2, Y)

Table 2. Obtained data of fermentation of glucose, maltose and maltotrioses [8]

Time (minus)	Maltose (M)	Glucose (G)	Maltotrioses (N)
0	13.1	13.10	13.10
10	10.8	11.0	10.63
20	8.5	8.15	7.9
30	7.0	7.10	6.78
40	5.4	5.55	5.13
50	4.2	4.35	3.9
60	3.7	3.9	3.38
70	3.0	3.25	2.65
80	2.4	2.20	1.93
90	1.9	2.25	1.50
100	1.6	2.0	1.18
110	1.25	1.7	0.80
120	1.0	1.5	0.5

Results and Discussion

Result Presentation

The results of the data collected, the test plots of the different models are as shown in table 2 below and figures 2, 3, 4, 5, 6, 7 and 8.

Table 3. Experimental results of fermentation of beer from Awonmama Brewery, Imo State, Nigeria.

Time (hrs)	Substrate (g/l)	Ethanol (g/l)	Biomass (g/l)
0	11.40	0	0.051
8	11.3	0.09	0.162
16	9.80	0.80	0.281
24	8.29	1.89	0.523
32	7.10	2.65	0.705
40	6.20	3.16	0.850
48	5.22	3.76	0.951
56	4.15	4.41	1.022
64	3.22	5.16	1.053
72	2.30	5.52	1.105
80	1.65	5.92	1.204
88	1.21	6.19	1.221
96	0.90	6.37	1.211
104	0.65	6.52	1.203
112	0.51	6.62	1.181
120	0.49	6.63	1.152

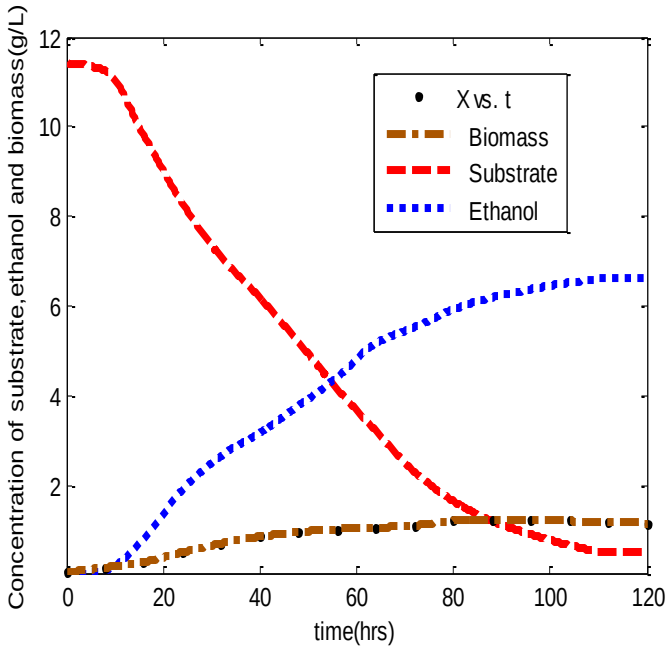

Figure 2.Concentrations of substrate, ethanol and biomass versus time (shape-preserving interpolant)

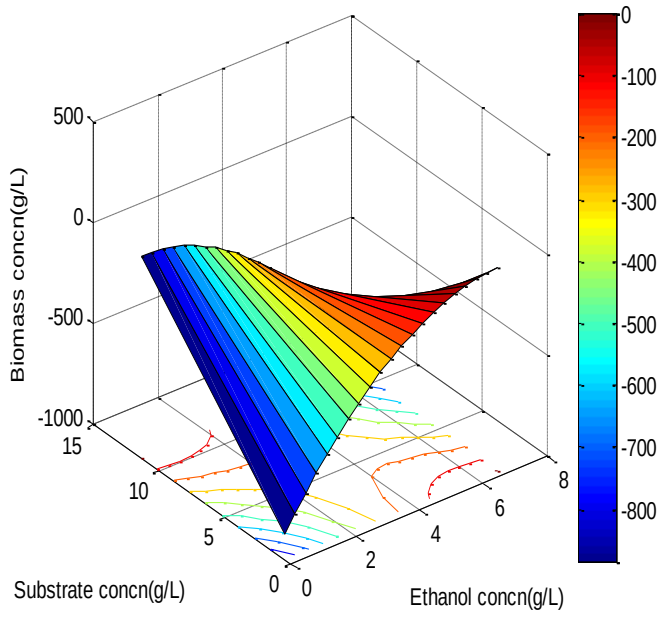

Figure 3. 3-D plot of biomass concentration versus substrate and ethanol during fermentation process (R^2=0.9936)

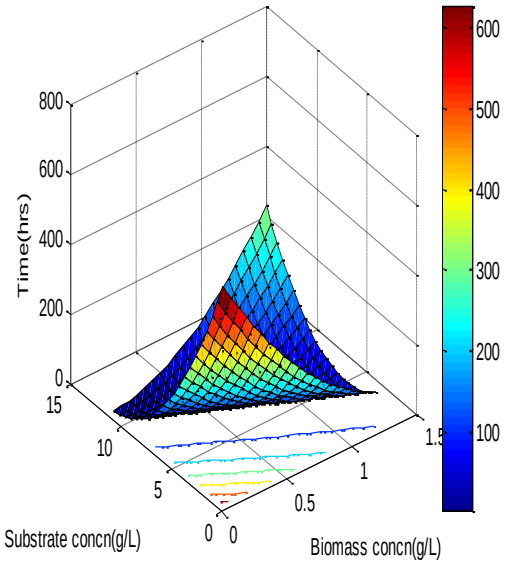

Figure 4. 3-D plot of fermentation time versus substrate and biomass concentrations (R^2=0.9980)

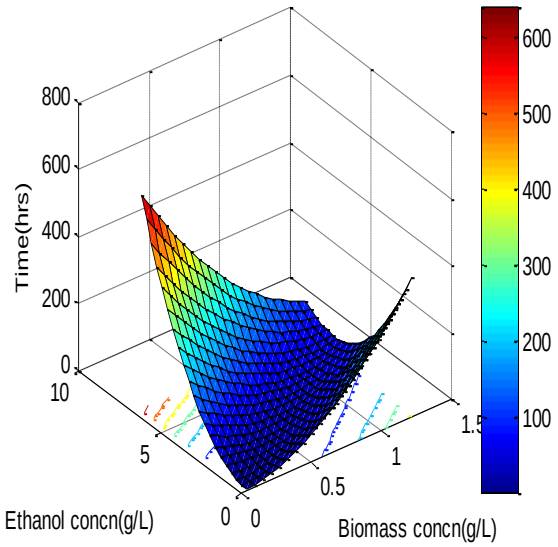

Figure 5. 3-D plot of fermentation time versus ethanol and biomass concentrations (R^2=0.9978)

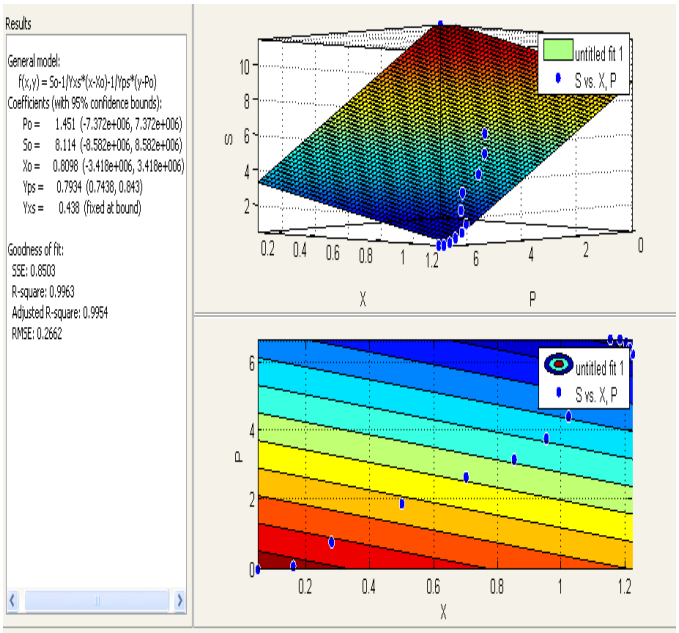

Figure 6. 3-D plot and cursor contour of substrate concentration versus biomass and product(ethanol) concentrations during fermentation; S=So-1/Yxs*(X-Xo)-1/Yps*(P-Po);R^2=0.9963.

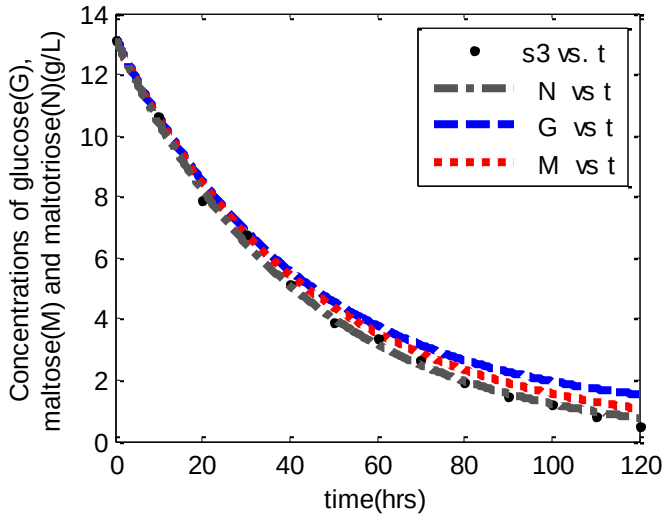

Figure 7. Concentrations of glucose, maltose and maltotriose versus time of fermentation

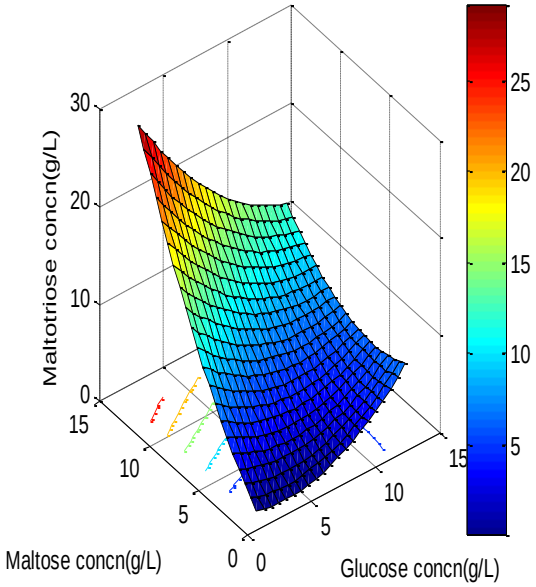

Fig. 8: Concentrations of maltotriose versus maltose and glucose during fermentation

Discussion

Figure 2 is the shape preserving interpolant plot of concentrations of substrate, ethanol and biomass against time. It shows the behaviour of these compounds during fermentation. As the substrate decreases, the production of biomass and ethanol increases at different degrees.

Figure 3 is the 3-D raw plot of surface response for biomass with substrate and ethanol. The curves on the floor show that there are different types of serious interaction between substrate and ethanol. The interactions are very serious because of the nature of curvatures on the floor. Note; if the lines are parallel to any of the floor, there is no interaction. If they are straight lines but coming from the origin it is directly proportional interaction. If the lines are parallel to the origin, it is inverse interaction but if the lines are curved, it is indeed a serious interaction.

Figure 4 is another 3-D response raw plot between time with substrate concentration and biomass concentration. The interaction on the floor between substrate concentration and biomass concentration is inverse and it is real to life.

Also, figure 5 is another 3-D response plot between time with ethanol and biomass concentration. The interaction on the floor is directly proportional, thus, real to life in fermentation process.

But from figure 6, where a 3-D plot of substrate, biomass and product (ethanol) was curve fitted with the model equation (10). MATLAB toolbox declared coefficients of the model at 95% confidence bound as;
$P_0 = 1.451$
$S_0 = 8.114$
$Y_{p/x} = 0.438$ i. e. 43.8%
$Y_{x/s} = 0.7934$ i. e. 79.34%
with R^2 of 0.9963. The percentage yield of ethanol (product) is higher (79.34%) than yield of biomass (43.8%). From the cursor contour (floor) of figure 6, production of ethanol (product is slightly inversely interacting with the production of biomass.

Figure 7 was made using model equations 2, 3 and 4. The models show that the three compounds were decreasing with time which is again real to life.

In figure 8 also, the 3-D surface response plot of maltotrioses concentration with concentrations of maltose and glucose are made. Thus, from the floor of figure 8, it is seen that there is serious interaction between concentration of maltose and that of glucose as we have parabolic curves during the fermentation process.

In summary, both models from Stoyan et al (2012) and Douglas and Fred (1994) were analytically solved to obtain their solutions. The analytical solutions of models from Stoyan et al (2012) and Douglas and Fred (1994) were used in curve-fitting the experimental data from fermentation process. Both showed very good correlation of $R^2 = 0.9963$. The adjusted R^2 (0.9954) does not deviate very much from

the R^2 of 0.9963 since there is no over parameterization in the models.

Conclusion

In this work, established models of renowned scholars of fermentation are analytically solved. Fermentation experiments were also performed on the production of ethanol and biomass from substrate (grain i.e. malted barley) with time and used to validate the analytical solutions of the scholarly models. The result shows that the models were real and true to life as they gave coefficient of correlation of 99.63%.

It is also observed that during this fermentation, there was serious interaction between substrate concentration and ethanol concentration, substrate concentration and biomass concentration. From the model, it was found that the yield of ethanol (product) was 79.34%, yield of biomass was 43.8%, initial ethanol before fermentation was 1.451g/lit. Substrate at the beginning S_0 = 8.114g/lit and initial biomass X_0 was 0.8098g/lit.

This result can be applied in fermentation planning in any brewing company or research centers to predict variation of certain parameters.

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