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CHEMICAL ENGINEERING

Optimization of the Performance of Packed Bed Fermentor with Immobilized Zymomonas Mobilis for the Production of Fuel Alcohol

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Abstract. Heterogeneous compartmental model is used to optimize the performance of a packed bed fermentor with immobilized zymomonas mobilis for the production of fuel alcohol. The results indicate that the outlet ethanol concentrations have maximum values that decreased with increasing feed sugar concentration at single bead diameter. The outlet ethanol concentrations have maximum values that increased with decreasing the dilution rate. As the dilution rate increased the ethanol production increased. As the substrate inhibition constant (K_I) increased both the maximum outlet ethanol concentration and the optimum feed sugar concentration increased up to K_I value of 500 g/L above that each have constant value.

Nomenclature

a	Specific area of bead	dm^{-1}
A	Cross sectional area of fermentor	dm^2
A_p	External surface area of a single floc	dm^2
A_s	External surface area of the bead	dm^2
A_{tf}	Total mass transfer area of flocs in a single capsule	dm^2
D_{es}	Diffusivities of sugar	dm^2/hr
D_{ep}	Diffusivity of ethanol	dm^2/hr

D_p	Floc diameter	dm
K_{gs}	Mass transfer coefficient for sugar through floc wall	dm/h
K_{gp}	Mass transfer coefficient for ethanol through the bead wall	dm/h
$\bar{K}_{gs}$	Mass transfer coefficient for sugar through the bead wall	dm/h
$\bar{K}_{gp}$	Mass transfer coefficient for ethanol through the bead wall	dm/h
K_I	Substrate inhibition constant	g/L
K_s	Saturation constant	g/L
K_p	Ethanol inhibition constant	g/L
K_p'	Rate constant	g/L
L	Fermentor length	dm
P	Ethanol concentration inside the floc	g/L
P_b	Ethanol concentration inside the bead	g/L
$\bar{P}_b$	Bulk ethanol concentration	g/L
P_{in}	Ethanol feed concentration	g/L
q	Volumetric flow rate	L/h
ϱ_c	Density of the bead	g/L
ϱ_f	Density of floc	g/L
r_p	Specific rate of ethanol production	g ethanol produced/ g dry wt biomass h
r_s	Specific rate of sugar consumption	g sugar cons./ g dry wt. biomass. h
r_x	Specific growth rate	g biomass prod./ g dry wt. biomass. h
S	Sugar concentration inside the floc	g/L
S_b	Sugar concentration inside the capsule	g/L
$\bar{S}_b$	Bulk sugar concentration	g/L
S_f	Sugar feed concentration	g/L
t	Time	h
μ_m	Maximum specific growth rate	h–1
V_c	Volume of the bead	L
V_p	Volume of a single floc	L
X	Biomass concentration	g dry wt./L
Y_c	Yield factor for yeast	g yeast produced/ g sugar consumed

Y_p	Yield factor for ethanol	g ethanol produced/ g sugar consumed

Introduction

The demand for ethanol increases yearly due to its important usage as alternative fuel, blend with gasoline in the production of gasohol or its many uses in industrial, medical and other fields [1].

Ethanol can be produced through the petrochemical route by the acid catalyzed hydration of ethylene or via the biochemical route where microorganisms (catalyst) are used with suitable substrates such as sugar, agricultural products or waste to produce ethanol.

Alcoholic fermentation takes place in different types of reactors such as batch, fed-batch and tower fermentors. The microorganisms which catalyze the fermentation reactions are either free in solution or immobilized inside different types of permeable beads (such as calcium alginate gel beads).

The production of ethanol in column type reactors packed with immobilized cells offers many advantages, such as, enhanced rate of ethanol production, due to high cell concentration and low product concentration. However, for the efficient design, optimization and control of this type of fermentor accurate and reliable design equations are necessary. The development of such models has been relatively slow and the models available are both mathematically complicated as well as unreliable.

Many investigators neglect the effect of the mass transfer resistance between the bulk of solution and the intracellular fluid on the rate of fermentation process [2]. Several investigators tried to develop reliable models for the immobilized packed bed fermentors [3-6]. Melick *et al.* [6] use the continuum models for the beads immobliliz-ing the cells, which borrow the effectiveness factor concept from gas-solid catalytic reactors. Recently El Nashaie *et al.* [7] develolped a compartmental model for the alcoholic fermentation process using immobilized whole cell in continuous tubular fermentors. The model was compared with a number of experimental runs and the superiority of the model was clearly demonstrated.

The objective of this paper is to use the compartmental model of El Nashaie *et al.* [7] to obtain the optimum performance of packed bed fermentor with immobilized zymomonas mobilis.

Mathematical Model

The compartmental heterogeneous model equations are developed for the flocs, the beads and the bulk of the fluid, see Fig. 1. For most of the cases the fluid flow in the bulk phase is considered to be in plug flow, while Melick *et al.* [6] considered an axial dispersion model for the bulk liquid phase and used the axial pelect number as an adjustable parameter.

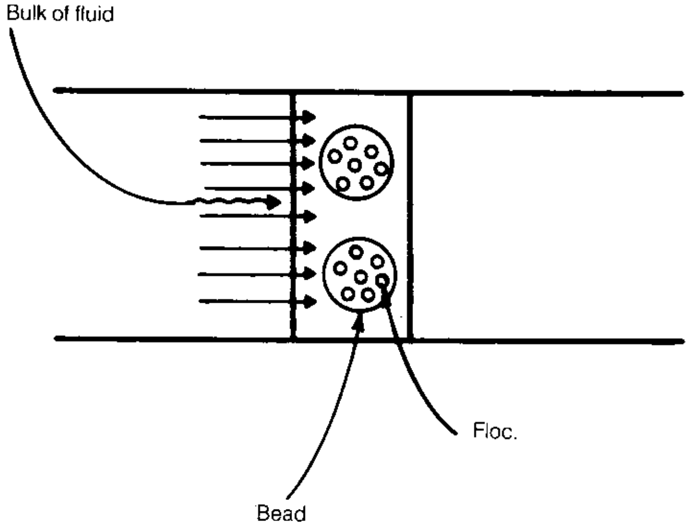

Fig. 1. **Cross section of the packed bed fermentor with immobilized whole cells**

Model Equations for Single Floc

Steady state substrate (sugar) mass balance for the floc gives:

$$A_p\, K_{gs}\, (S_b - S) = r_s\, \varrho_f\, V_p \tag{1}$$

where r_s is the specific rate of sugar consumption [7, 8]

$$r_s = \frac{\mu_m\, K_p\, S}{Y_c (K_p + P)\,[(K_s + S) + S^2/K_I)]} + \frac{\mu_m\, K_p^`}{Y_c\,(K_p^` + P)} \tag{2}$$

By considering the flocs shape to be spherical, we get $A_p / V_p = 6/D_p$ where D_p is the equivalent diameter of the floc. Equation (1) can now be written as

$$[6\,K_{gs}\,(S_b - S)/D_p] - r_s\,\varrho_f = 0 \tag{3}$$

Ethanol mass balance for the floc can be written in similar manner as equation (3) to give

$$[-6\,K_{gp}\,(P - P_b)/D_p] + r_p\,\varrho_f = 0 \tag{4}$$

For unstructured models, $r_p = r_s\,y_p$, is always valid, however, y_p changes from one strain to the other. So equation [4] can be rewritten as:

$$[-6\,K_{gp}\,(P - P_b)/D_p] + r_s\,y_p\,\varrho_f = 0 \tag{5}$$

The biomass concentration is assumed to change linearly with the length of the fermentor and is expressed by the following equation

$$X = \bar{a}\,L + b \tag{6}$$

where X is the cell concentration, L is the distance along the length of the fermentor, ā and b are constant.

The concentration of microorganism X* was positively measured by Melick *et al.* [6] at lenglth L* and thus this point must be on our straight line, and therefore we get

$$\bar{a} = X^* - \bar{a}\,L^* \tag{7}$$

and

$$X = X^* + \bar{a}\,(L - L^*) \tag{8}$$

Therefore, the variation of the microorganism with the length of the fermentor depends only on one parameter (ā).

The validity of this assumption has been asserted from previous work [7], where using such a linear profile improved the model prediction considerably.

Model Equations for the Bead

Substrate (sugar) mass balance for the bead gives:

$$A_s\,\bar{K}_{gs}\,(\bar{S}_b - S_b) = A_{tf}\,K_{gs}\,(S_b - S) \tag{9}$$

Ethanol mass balance gives:

$$A_s\,\bar{K}_{gp}\,(P_b - \bar{P}_b) = A_{tf}\,K_{gp}\,(P - P_b) \tag{10}$$

where $A_{tf} = 6\,(X)\,Vc/\,\varrho_f\,D_p$

The mass transfer resistance inside the bead is lumped into a hypothetical film at the external boundary of the bead. The values of the mass transfer coefficient are obtained by assuming a parabolic profile concentration inside the bead and using a one point internal collocation approximation [9].

$$\bar{K}_{gs} = \frac{D_{es} \text{ X } 3.5}{R_{cap}} \tag{11}$$

$$\bar{K}_{gp} = \frac{D_{ep} \text{ X } 3.5}{R_{cap}} \tag{12}$$

Where D_{es} and D_{ep} are the diffusivities of sugar and ethanol in the bead respectively. R_{cap} is the bead radius.

The diffusion coefficient in the calcium-alginate was measured by Tanaka *et al.* [10], Bevia *et al.* [11] and Nagashima *et al.* [12].

In addition to those parameters, the density of the bead containing the flocs was found experimentally to be 1081.08 g/L. The density was measured experimentally by finding the displaced volume of a specific weight of beads. The beads were formed by adding the microorganism to sodium alginate, then using a syring, a drop wise of the homogeneous microorganism-sodium algninate was added to a stirred calcium chloride solution (beads immobilizing the microorganism were formed).

Overall Reactor Model

The differential equations describing the change of sugar and ethanol concentration along the length of the packed bed fermentor are obtained by taking a differential element along the length of the fermentor. For sugar we obtain

$$q \bar{S}_b = q (\bar{S}_b + \Delta \bar{S}_b) + a A \Delta L \bar{K}_{gs} (\bar{S}_b - S_b) \tag{13}$$

taking the limits as $\Delta L \xrightarrow{\quad} O$ and $\Delta S_b \xrightarrow{\quad} O$. Equation (13) becomes:

$$d\bar{S}_b/dl = - aA/q \bar{K}_{gs} (\bar{S}_b - S_b) \tag{14}$$

Similarly for ethanol we get

$$d\bar{P}_b/dl = aA/q \bar{K}_{gp} - \bar{P}_b) \tag{15}$$

System parameters used in this model (compartmental model) are summarized in Table 1.

Table 1. Model parameters [8]

Parameter type	Parameter symbol	Parameter value
Kinetic	μ_m	0.429 h–1
	K_p	70 g/L
	K_s	1.7 g/L
	K_I	726.75 g/L
	K'_p	3 g/L
	Y_c	0.52 dimensionless
	Y_p	0.48 dimensionless
Physical	D_p	2.5 × 10–4 dm
	K_{gs}	5.04 × 10–2 dm/h
	K_{gp}	1 × 10–3 dm/h
	D_{es}	9.36 × 10–5 dm^2/hr
	D_{ep}	17.21 × 10–5 dm^2/hr
	ϱ_f	200 g/L
	ϱ_c	1081.08 g/L
	$\bar{K}_{gs}$	Eq.11
	$\bar{K}_{gp}$	Eq. 12
	$\bar{a}$	–0.055
	L^*	4.15 dm
	X^*	0.12 g/L

Results and Discussion

It is desired industrially in any production process to find the optimum operating conditions that yield the maximum product concentration and production rate. The heterogeneous compartmental model is used to find the effect of the operating conditions on the performance of an experimental fermentor that has a length of 8.3 dm and diameter of 0.174 dm, the fermentor is divided into 166 steps in the axial direction and the outlet ethanol concentration and production are obtained by solving the algebraic equations developed.

Effect of capsule diameter

Figure 2 shows that the outlet ethanol concentration has a maximum value at single capsule diameter of 0.02 dm for different feed sugar concentrations. The value of the maximum ethanol concentration decreases as the feed sugar concentration increases.

The maximum outlet ethanol concentration obtained is due to the non-monotonic dependence of the rate of reaction upon sugar concentration. Fig. 3 shows such dependence under different levels of outlet ethanol concentration. Obviously as the ethanol concentration increases, the whole curve is shifted towards lower rates of reaction. However, the non-monotonic behaviour can be observed for all levels of ethanol concentration.

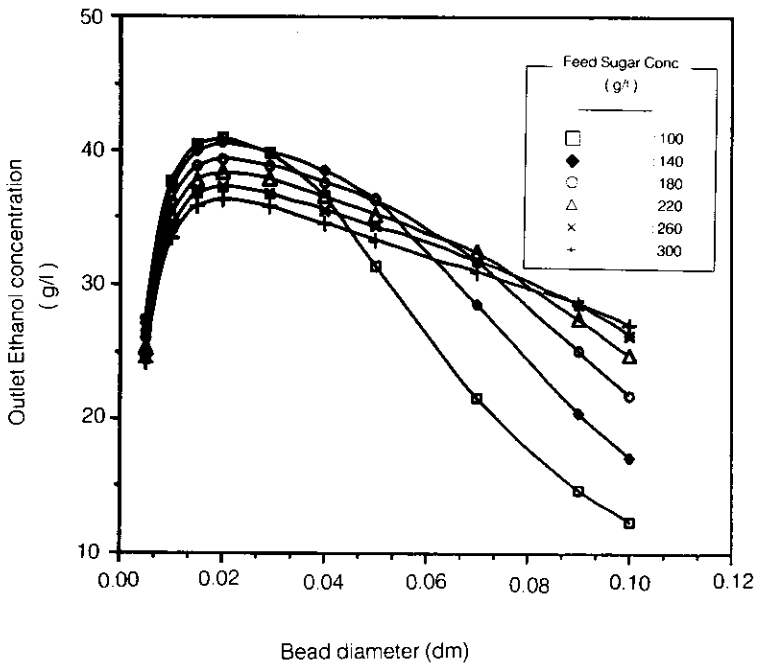

Fig. 2. Effect of bead diameter on the outlet ethanol concentration

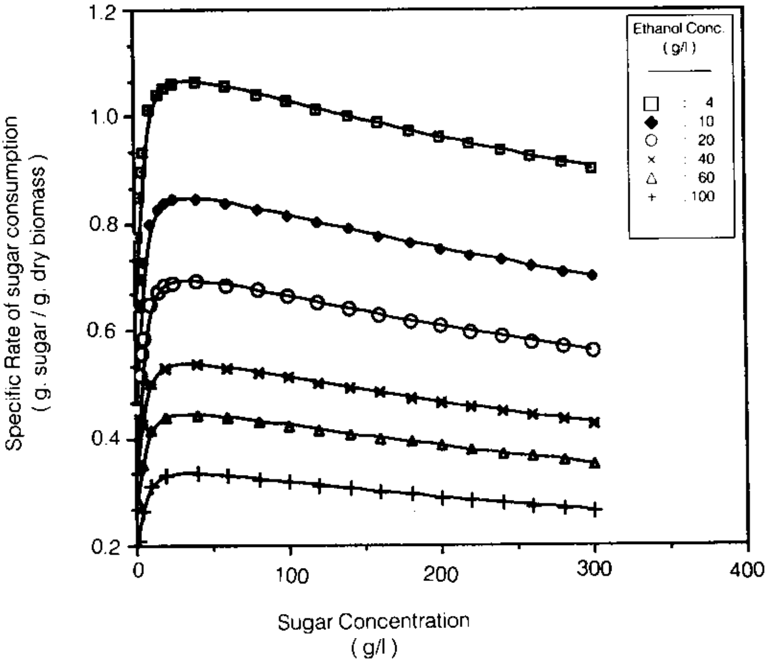

Fig. 3. **Effect of ethanol concentration on the dependence of the specific rate of sugar concentration**

Effect of feed sugar concentration

The outlet ethanol concentration show maximum values at different dilution rates with changing feed sugar concentration (Fig. 4). The maximum outlet ethanol concentration values increase as the dilution rates decrease. As the dilution rate increased from 0.3 to 1.2 hr^{-1} the maximum outlet ethanol concentration values lie in the feed sugar concentration range of 190 to 100 (g/l) respectively. Table 2 shows the feed sugar concentrations at which maximum outlet ethanol concentration occurs at different dilution rates. Similarly, Fig. 5 indicates that the outlet ethanol concentration shows maximum values as the feed sugar concentration is increased at different substrate inhibition constant (K_I). Different strains have different inhibition tendencies and hence have different corresponding values of K_I's. The effects of changing K_I value is shown in Fig. 5, where increasing K_I increases the maximum outlet ethanol concentration.

The maximum outlet ethanol concentration values correspond to the feed sugar concentration of 45 to 140 (g/l) as the K_I values change from 0.85 to 726.75 (g/l) respectively.

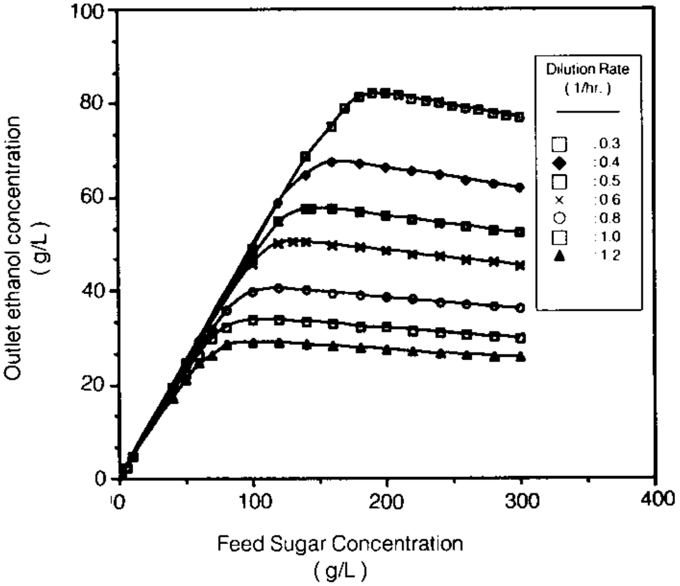

Fig. 4. Effect of feed sugar concentration on outlet ethanol concentration at different dilution rate
D_{cap} = 0.029 dm K_1 = 726.75 g/l

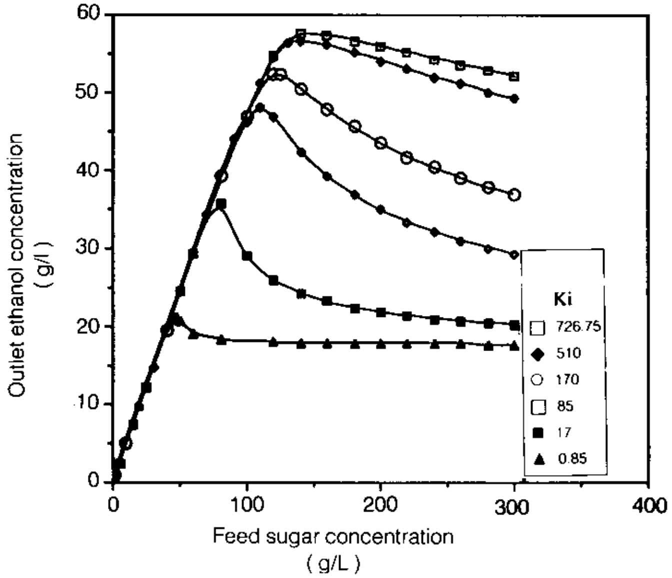

Fig. 5. Effect of feed sugar concentration on the outlet ethanol concentration at different value of saturation constant
Dilution rate $= 0.5\ hr^{-1}$ $D_{bead} = 0.029$ dm

Effect of dilution rate

The dilution rate is the reciprocal of the residence time, so as the dilution rate increases the residence time decreases. Fig. 6 indicates that as the dilution rate increases the outlet ethanol concentration decreases due to the decrease of the residence time. The effect of dilution rate on ethanol production rate is shown in Fig. 7 where no maximum is observed, as the dilution rate increases the ethanol production rate also increases, for all feed sugar concentrations investigated. The flow rate should obviously not go lower than certain levels, otherwise additional mass transfer and CO_2 blanketing will occur.

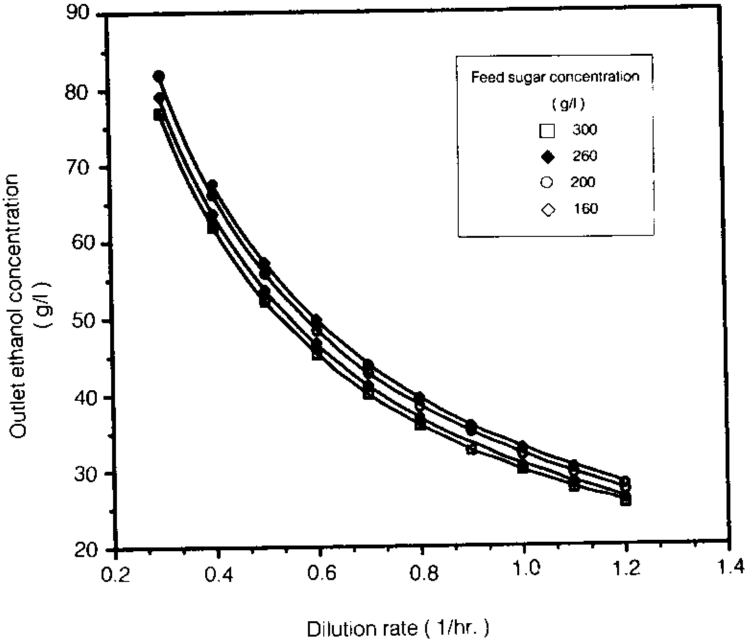

Fig. 6. **Effect of dilution rate on outlet ethanol concentration**

Effect of strength of substrate inhibition

Figure 5 shows that as K_I increases, the maximum ethanol concentration values corresponding to the optimum feed sugar concentrations increases sharply, then reaches almost constant value of 56.72 g/l beyond K_I value of 500 g/L, which is shown clearly in Fig. 8 where the maximum outlet ethanol concentration reaches a plateau beyond K_I value of 500. The change in the optimum feed sugar concentration, which is the feed sugar concentration for the maximum outlet ethanol concentration, with

K_I is shown in Fig. 9. Increasing the K_I value increases the optimum feed sugar concentration sharply at the beginning, then reaches a constant value at K_I value of 500; any more increase in the K_I value has no effect on the optimum feed sugar concentration which reaches constant value of 140 g/l.

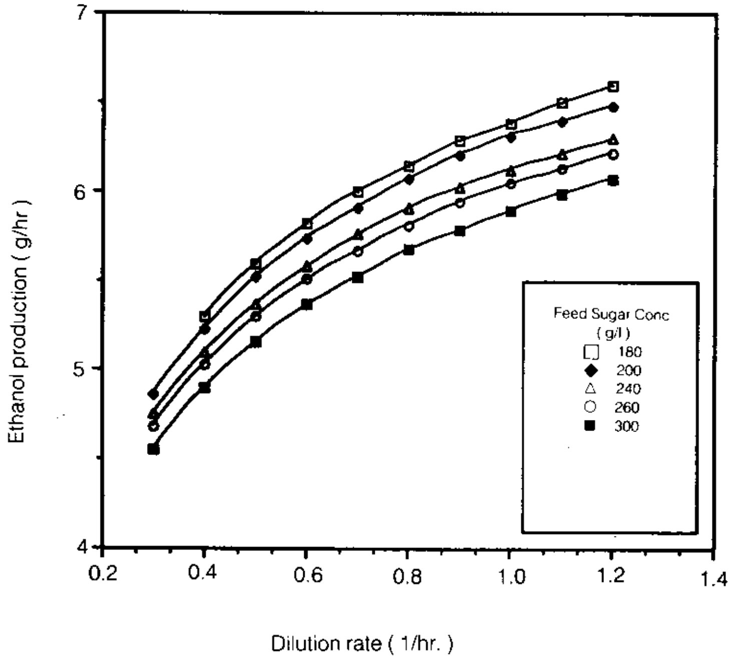

Fig. 7. **Effect of dilution rate on ethanol production of different feed sugar concentration**

Conclusion

A heterogeneous compartmental model is used to optimize the performance of a packed bed fermentor with immobilized zymomonas mobilis. The fermentor was divided into 166 compartments and for a known feed sugar concentration to the fermentor. The outlet ethanol concentration and the production rate from the fermentor are predicted under different operating conditions such as bead diameter, dilution rate and different substrate inhibition constant. It was found that the outlet ethanol concentrations have maximum values which decrease with the increase of feed sugar concentration at single bead diameter of 0.02 dm.

The outlet ethanol concentration shows a maximum value as the feed sugar concentration increases at a specific dilution rate. As the dilution rate decreases the maximum value of the outlet ethanol concentration increases.

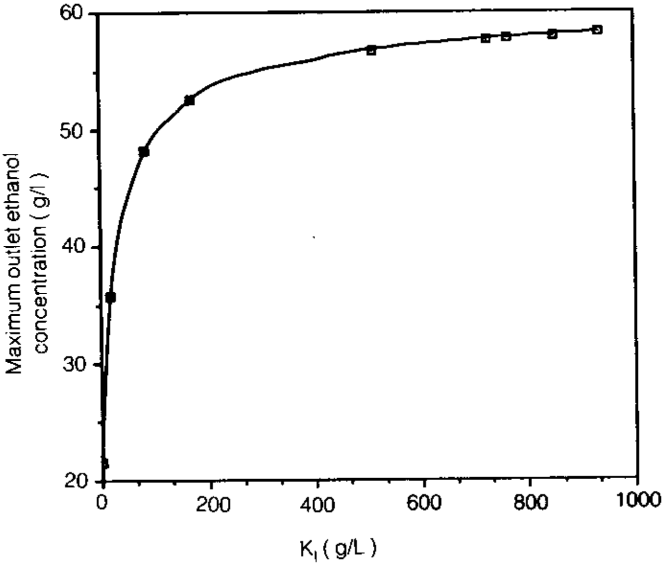

Fig. 8. Effect of K_I on max. outlet ethanol concentration

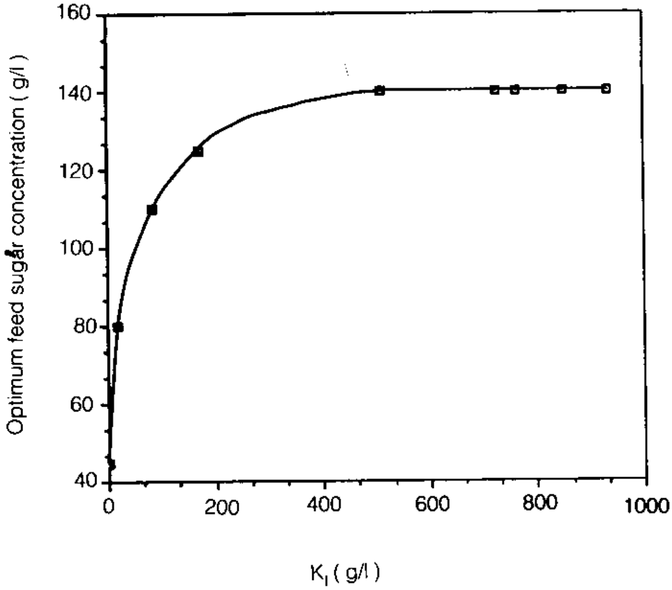

Fig. 9. Change of the optimum feed concentration with K_I

The maximum outlet ethanol concentration increased sharply at low substrate inhibition constant as the feed sugar concentration increased until it reaches almost constant value of 56.72 g/1 at K_I = 500 g/L. The optimum feed sugar concentration increased as K_I increased from 0.85 to 500 g/L above that the optimum feed sugar concentration reaches a constant value of 140 g/l. The dilution rate shows no maximum for ethanol production rate.

The packed bed fermentor will be operated under optimum condition by selecting a bead diameter of 0.02 dm, feed sugar concentration of 140 g/L and dilution rate of 0.5 hr^{-1} (Table 2).

Table 2. Feed sugar concentration at which maximum outlet ethanol concentration occurs at different dilution rate

Dilution rate 1/hr	Feed sugar concentration (g/L)	Maximum outlet ethanol concentration (g/L)
0.3	190	82.0865
0.4	160	67.4892
0.5	145	57.6452
0.6	130	50.3583
0.7	120	44.761
0.8	120	40.3403
0.9	100	36.66
1.0	100	33.7716
1.1	100	31.989
1.2	100	29.1311

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أمثلية أداء مُخَمّر ذو مهد ثابتة من الزيمومنيس موبلس المقيدة الحركة لإنتاج الوقود الكحولي

أنيس حمزة فقيها

قسم الهندسة الكيميائية، كلية الهندسة، جامعة الملك سعود، ص.ب ٨٠٠،
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(استُلم في ١٥/٥/١٩٩١م؛ قُبل للنشر في ٣٠/٩/١٩٩١م)

ملخص البحث. استخدم نموذج مرحلي غير متجانس لإيجاد أفضل ظروف أداء مُخَمّر ذو مهد ثابتة من الزيمومنيس موبلس المقيدة الحركة لإنتاج الوقود الكحولي. دلت النتائج على أن تركيز الإيثانول الخارج من المفاعل يصل إلى قيم عالية تتناقص بزيادة تركيز السكر الداخل عند قيمة ثابتة لقطر الكريات الحاوية للزيمومنيس موبلس. كذلك فإن تركيز الإيثانول الخارج من المفاعل يزداد بنقص معدّل التخفيف، وأنه كلما زيد في معدّل التخفيف فإن إنتاجية الإيثانول تزداد. وقد أشارت النتائج إلى أنه بزيادة قيم ثابت تبطىء مواد التفاعل فإن كل من القيم العالية للإيثانول الخارج من المفاعل وكذلك القيم المثلى لتركيز السكر الداخل للمفاعل تزداد حتى تصل قيمة الثابت إلى ٥٠٠ جرام/ لتر وبعد ذلك فإن كلتا القيمتين تصل إلى قيمة حدّية ثابتة كل على حدة.