



Research Article

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Reactor design strategy: Production of xanthan from sugarcane broth

A. Arumugam, P. Vignesh and V. Ponnusami

School of Chemical & Biotechnology, SASTRA University, Thirumalaisamudram, Thanjavur, India

ABSTRACT

Xanthan gum is exo-polysaccharide, produced by Xanthomonas campestris. Considering a reactor operating in continuous mode, optimum dilution rate is determined by maximization condition. Optimum dilution rate is the dilution rate at which the productivity of xanthan gum is maximum. The current work is focused on implementing an algorithm for design of reactor, having optimum dilution rate as the operating condition. The steps of the algorithm and values obtained are briefed in this paper.

Keywords: Xanthan gum, Mathematical Model, Reactor Design, Optimum Dilution rate, Heat Transfer

INTRODUCTION

Xanthan gum is an industrial grade biopolymer, used as a rheology modifier. It is produced by Xanthomonas campestris, as an exo-polysaccharide in its slime. It is a gram negative bacterium[1].

Vignesh et. al., (2015) reported the mathematical modeling and steady state simulation of Xanthan gum production, using sugarcane broth as substrate [2]. Logistic equation for cell growth and Leudeking-Piret equation for substrate consumption and product formation were taken into account for developing mathematical model. The obtained reactor engineering model was simulated to determine the optimum dilution rate.

Two modes of continuous operation were considered:

1. Without Cells' Recycling
2. With Cells' Recycling

The mathematical models for predicting the behaviors of substrate consumption, biomass and product formation were formulated with the assumptions of well-mixed, aerated fermentation system and steady state, isothermal operation.

For case of simplicity, reactor design will be dealt only for first mode of operation (without recycling of cells). The model equations as reported,

Biomass Concentration in the outlet stream is given by,

$$X = Y_{XS} S_0 \left(1 - \frac{D}{\mu_m}\right)$$

Substrate Concentration in the outlet stream is given by,

$$S = \left(S_0 - \frac{X}{Y_{XS}}\right)$$

Product Concentration in the outlet stream is given by,

$$P = Y_{PX} X$$

The productivity of biomass is given by, $P_X = D X$

The productivity of product is given by, $P_p = D P$

The kinetic parameters required are for the optimized media with inlet sucrose concentration 27 g/L [3].

The kinetic parameters are $\mu_m = 0.411 \text{ hr}^{-1}$, $Y_{XS} = 0.725 \text{ g of biomass/g of substrate}$, $Y_{PX} = 0.881 \text{ g of xanthan gum/g of substrate}$

The dilution rate at which the maximum productivity occurs is the optimum dilution (D_{opt}) to operate the reactor.

At D_{opt} , $\frac{d(P_X)}{dD} = 0$ and $\frac{d^2(P_X)}{dD^2} < 0$ (36) where $P_X = D X$ $D_{opt} = \frac{\mu_m}{2} = 0.205 \text{ hr}^{-1}$

Design Strategy

The design of the reactor is based on volumetric mass transfer coefficient of oxygen, $k_L a$ and optimum dilution rate at which the reactor is to be operated. The target $k_L a$ is calculated assuming the steady state between oxygen mass transfer and oxygen consumption by the cells.

$$k_L a = \frac{\mu Y_{O_2 X} X}{(C^* - C)}$$

The algorithm of Reactor Design is as follows,

1. Assume H/D Ratio. Calculate D for the given working volume
2. For the type of impeller to be used (D_t/D_i), Calculate D_i
3. Assume tip speed ($\Pi N_i D_i > 2.5$), Calculate N_i
4. Choose the velocity of inlet air, $V_g < 120 \text{ m/hr}$
5. For the assumed conditions, flooding is checked. If the impeller flooding is found, goto 3 or 4
6. Calculate Impeller Reynold Number
7. Calculate Ungassed Power [4].
8. Calculate corrected gassed power. (using correction factor, F_C)
9. Determine the number of impeller sets
10. Calculate Actual ungasged power
11. Find P_g / P_3
12. Calculate Gassed Power
13. Calculate $k_L a$ of the designed reactor
14. Check Design $k_L a \geq$ Target $k_L a$. If not, goto 3 or 4.

Target $k_L a$

The critical oxygen concentration to be maintained at Production phase is 6 % -10 % saturation [5].

For water and dilute solution, solubility of oxygen is given by,

$$C_{AL}^* = 14.161 - 0.3943 T + 0.0077147 T^2 - 0.0000646 T^3 \frac{\text{mg}}{\text{L}}$$

where T in $^{\circ}\text{C}$

At 28 $^{\circ}\text{C}$, $C_{AL}^* = 0.781 \text{ mg/L}$.

$$Y_{O_2 X} = \frac{14.59 \text{ mmol of } O_2}{\text{g of biomass}} = 0.47 \frac{\text{g of } O_2}{\text{g of biomass}} \quad [6]$$

Table 1: $k_{L a, \text{target}}$ for different Critical O_2 saturation

Critical O_2 Saturation (%)	$k_{L a, \text{target}} (\text{s}^{-1})$
5	0.0356
10	0.0376
25	0.0451

Reactor Design

Working Volume = 15 m^3 and Rushton turbine is assumed.

Volume of the cylindrical vessel = $\Pi D_t^4 H_L / 4$.

$D_t = 2.136 \text{ m}$; $H_L = 4.186 \text{ m}$

$D_t / D_i = 3 \rightarrow D_i = 0.712 \text{ m}$

$\Pi N_i D_i > 2.5 \rightarrow N_i = 2.5 \text{ rps} \rightarrow \Pi N_i D_i = 5.59 \text{ m/s}$

Impeller Reynold's number: $N_{Rei} = N_i^{2-n} D_i^2 \rho / k^{n-1}$. K
 $K = 42.85 \text{ dyne s}^n / \text{cm}^2 = 4.285 \text{ Pa s}^n$ [7]
 $n = 0.29$
 $k = 10$ for Rushton Turbine
 $N_{Rei} = 2950.89$

For $N_{Rei} = 2950.89$, Power number is $N_p = 6$.
 Ungassed power, $P_1 = N_p \rho N_i^3 D_i^5 = 17.411 \text{ kW}$

$$\text{Correction Factor, } F_c = \sqrt{\frac{\left(\frac{D_t}{D_i}\right)\left(\frac{H_L}{D_i}\right)}{\left(\frac{D_t}{D_i}\right)^* \left(\frac{H_L}{D_i}\right)^*}}$$

Standard dimensions, $(D_t/D_i)^* = 3$; $(H_L/D_i)^* = 3$
 $F_c = 1.4$; Corrected Ungassed Power, $P_2 = F_c * P_1 = 24.375 \text{ kW}$

$$P_3 = n_i * P_2$$

$$\frac{H_L - D_i}{D_i} > n_i > \frac{H_L - 2 D_i}{D_i}$$

$n_i = 4 \rightarrow P_3 = 97.5 \text{ kW}$ (Actual Ungassed Power)

An expression for the ration of gassed to ungassed power as a function of operating conditions [8].

$$\frac{P_g}{P_3} = 0.1 \left(\frac{Q_g}{N_i V}\right)^{-0.25} \left(\frac{N_i^2 D_i^4}{g W_i V^{\frac{2}{3}}}\right)^{-0.2}$$

Air flow rate is, $Q_g = V_g A$.

Assume, $V_g = 70 \text{ m/hr}$

$$Q_g = 0.06967 \text{ m}^3/\text{s}$$

Flooding occurs at $0.2198 \text{ m}^3/\text{s}$ for given conditions. $\left(0.6 \left(\frac{N_i^2 D_i^5}{D_t^{2.5}}\right)\right)$

$k_L a$ is given by [9],

$$k_L a = \frac{0.033}{D_t^4} \left(\frac{P_g}{V}\right)^{0.541} Q_g^{\frac{0.541}{\sqrt{D_t}}} = 0.055 \text{ s}^{-1} > \text{Target } k_L a$$

$$\text{Gas hold up, } \phi = \frac{V_T - V_L}{V_T}$$

$$\phi = 1.8 P_m^{0.14} V_g^{0.75} \text{ where } P_m = \frac{P_g}{\rho V_L}$$

$$\phi = 0.1147; V_T = 16.9434 \text{ m}^3 \rightarrow H_L^* = 4.7283 \text{ m}$$

Including 10% allowance, $H_L^{**} = 5.2 \text{ m}$

Design of Heat Transfer system

Heat released during the process, $Q = -\Delta H_{rxn} + W_s + W(\text{heat dissipated by sparging})$ [10]

$$-\Delta H_{rxn} = q_{O_2} \times \left(460 \frac{\text{kJ}}{\text{gmol of } O_2}\right)$$

$$q_{O_2} = \mu Y_{O_2 X} X$$

$$-\Delta H_{rxn} = 56.62 \text{ kW}$$

$$W_s = P_g = 65.325 \text{ kW}$$

W - Heat dissipated by agitation

$$\text{Assuming isothermal expansion of gas, } -W = RT \ln \left(\frac{P_1}{P_2}\right)$$

The negative sign denotes the heat is dissipated into the fermentation broth [11].

Assuming the inner pressure is 3 times the inlet pressure of air.

$W = 2758.4265 \text{ J/gmol of O}_2$
 Air flow rate = $0.06967 \text{ m}^3/\text{s}$

Assuming inlet air behaves ideally,
 $PV = nRT$

$$\frac{n}{V} = \frac{112589}{8.314 * 302} = 44.84 \frac{\text{gmol}}{\text{m}^3}$$

$$Q_g = 3.124 \text{ gmol/m}^3$$

$$W = 8.167 \text{ kW}$$

$$Q = 56.62 + 65.325 + 8.617 = 130.562 \text{ kW}$$

We know that, $Q = m' C_p \Delta T$,

where m' is the mass flow rate of cooling water, C_p is the specific heat capacity of cooling water

$$C_p = 4.186 \text{ kJ/kg.K}$$

$$m' \Delta T = 31.19 \text{ kg K/s}$$

Assuming, $\Delta T = 10 \text{ K}$ ($T_1 = 10 \text{ }^\circ\text{C}$, $T_2 = 20 \text{ }^\circ\text{C}$)

Hence, $m' = 3.119 \text{ kg/s}$

The relation between overall and individual heat transfer coefficients is given by,

$$\frac{1}{U} = \frac{1}{h_i} + \frac{1}{h_o} + \frac{x}{K} + \frac{1}{h_{f_i}} + \frac{1}{h_{f_o}}$$

Correlations for individual heat transfer coefficients [12]

For Baffled vessel, $N_{Rei} > 400$

$$Nu = 0.54 N_{Rei}^{0.67} N_{Pr}^{0.33} \left(\frac{\mu}{\mu_w} \right)^{0.14}$$

and, $Nu = \frac{h_i d_i}{k_f}$ and k_f is the thermal conductivity of fermentation broth

Jacket side heat transfer coefficient is given by Ditter's Bolter equation,

$$Nu = 0.023 N_{Re}^{0.8} N_{Pr}^{0.4}$$

and, $Nu = \frac{h_o d_o}{k_{water}}$

Average Molecular weight

Table 2: Molecular Formula of Components

Component	Molecular Formula
Biomass	$\text{CH}_{1.79}\text{O}_{0.5}\text{N}_{0.2}$
Sucrose	$\text{C}_{12}\text{H}_{22}\text{O}_{11}$
Xanthan gum (Monomer)	$\text{C}_{35}\text{H}_{49}\text{O}_{29}$

Table 3: Calculation of Mole Fraction of components in fermentation broth

Component	Concentration (g/L)	Specific weight (g/kg)	Mass fraction	Molecular weight (g/gmol)	Basis: 1 kg	Mole fraction
					No. of moles	
Biomass($\text{CH}_{1.79}\text{O}_{0.5}\text{N}_{0.2}$)	9.81	9.66	$9.66 * 10^{-3}$	24.9	0.388	$7.138 * 10^{-3}$
Substrate (Sucrose)	13.46	13.26	0.0132	342	0.03879	$7.1369 * 10^{-4}$
Product(Xanthan gum)	7.95	7.83	$7.83 * 10^{-3}$	933 (Monomer)	0.08429	$1.55 * 10^{-3}$
Oxygen	$7.75 * 10^{-3}$	$7.63 * 10^{-3}$	$7.69 * 10^{-6}$	32	$2.386 * 10^{-4}$	$4.3899 * 10^{-6}$
Water	-	969.2	0.96	18	53.84	0.9905

Average Molecular Weight is, $M = \sum x_i M_i = 19.6971$

Specific Heat Capacity

Water (liquid):

$$C_p = C_1 + C_2 + C_3 T^2 + C_4 T^3 + C_5 T^4$$

Oxygen (gas):

$$C_p = C_1 + C_2 T + \frac{C_3}{T^2}$$

Table 4: Empirical constants (Water and Oxygen) for determination of Specific heat capacity

Component	C1	C2	C3	C4	C5
Water	276370	-2090.1	8.125	-0.014116	9.3701*10 ⁻⁶
Oxygen	8.27	0.000258	-187700		

Specific heat capacity (@ 28 °C) of biomass and Xanthan gum are predicted by Kopp's rule.

Table 5: Specific Heat Capacity of Components in Fermentation broth

Component	Specific Heat Capacity (kJ/kg.K)
Water	4.184
Oxygen (gas)	0.8227
Biomass (solid)	1.5548
Sucrose (solid)	1.2599
Xanthan gum (solid)	1.3046

Specific Heat Capacity of fermentation broth is calculated using mixture rule,

$$C_{p_{mix}} = \sum x_i C_{p_i} = 4.097 \text{ kJ/kg.K}$$

where x_i is the mass fraction of the components when C_{p_i} is expressed in kJ/kg.K,

x_i is mole fraction of the components when C_{p_i} is expressed in kJ/kmol.K

Thermal Conductivity

The thermal conductivity of liquids is given by Weber equation, $k = 3.56 * 10^{-6} C_p \left(\frac{\rho^4}{M}\right)^{\frac{1}{4}}$

$k = 0.55 \text{ W/m.K}$

Thickness of Reactor Vessel

Thickness, $t = \frac{P_i D_i}{2 J f - P_i}$ where, P_i is the design pressure; D_i is the diameter of vessel; J is the joint efficiency

(usually 0.85 for double welded pressure vessel)

Mass flow rate of water = 3.119 kg/s

Volumetric Flow rate of water = $3.119 * 10^{-3} \text{ m}^3/\text{s}$

$d_e = 0.06 \text{ m} \rightarrow$ Velocity of Cooling water = 0.81 m/s

Permissible shear stress, $f = 135 \text{ N/mm}^2$ for Carbon steel (AISI1020)

Thickness, $t = 1.048 \text{ mm}$

Minimum Corrosion Allowance = 2 mm

Hence, $t = 3.048 \text{ mm}$

Minimum Practical Thickness (from design data) for vessel diameter of 2-2.5 m is 9 mm

So, $x = 9 \text{ mm}$ and $k = 54 \text{ W/m.K}$

Heat Transfer Coefficients

Table 6: Values of Heat Transfer Coefficient

Heat Transfer Coefficient	Value (W/m ² .K)
h_i	423.463
h_o	3442.26
h_{fi}	5000
h_{fo}	7500
U	317.26

Determination of Heat Transfer Area

Logarithmic Mean Temperature difference, $\Delta T_{LMTD} = \frac{\Delta T_1 - \Delta T_2}{\ln\left(\frac{\Delta T_1}{\Delta T_2}\right)} = 13.38 \text{ K}$

$$A = \frac{Q}{U \Delta T_{LMTD}} = 30.757 \text{ m}^2$$

$$A = \Pi d_0 L \rightarrow L = 4.564 \text{ m}$$

CONCLUSION

Having known the reaction kinetics of xanthan gum fermentation from Sugarcane broth, the mathematical model was developed, which was simulated to determine the optimum dilution rate. For the optimum dilution rate of 0.205 hr^{-1} , the reactor design algorithm as given above was implemented to determine the design and operating parameters, based on $k_{L,a}$. Design was based on mass transfer coefficient; hence the possibility of mass transfer being a rate limiting step is eliminated. None of the transport phenomena will be rate limiting, in this design, as the calculation of optimum dilution rate was based on reaction kinetics.

Partial List of symbols (remaining explained as used)

V_L	Working volume of fermentor, m^3
D	Dilution rate, hr^{-1}
D_{opt}	Optimum dilution rate, hr^{-1}
μ	Specific growth rate, hr^{-1}
μ_m	Maximum specific rate, hr^{-1}
X_0	Concentration of biomass in inlet stream, kg m^{-3}
X	Concentration of biomass in outlet stream, kg m^{-3}
X_m	Maximum biomass concentration (i), kg m^{-3}
S_0	Concentration of substrate in inlet stream, kg m^{-3}
S	Concentration of substrate in outlet stream, kg m^{-3}
P_0	Concentration of Product in inlet stream, kg m^{-3}
P	Concentration of Product in outlet stream, kg m^{-3}
P_x	Productivity of biomass, $\text{kg m}^{-3}\text{hr}^{-1}$
P_p	Productivity of product, $\text{kg m}^{-3}\text{hr}^{-1}$
$k_{L,a}$	Volumetric Mass transfer coefficient, s^{-1}
C^*	Equilibrium Oxygen Concentration (Solubility of Oxygen) in fermentation broth, kg/m^3
C_{crit}	Critical Oxygen Concentration in fermentation broth, kg/m^3
C	Oxygen Concentration in fermentation broth, kg/m^3
k	Thermal Conductivity of fermentation broth, W/m.K
k'	Thermal Conductivity of metal wall, W/m.K
x	Thickness of metal wall, m
h_i	Heat Transfer Coefficient of Fermentation broth side, $\text{W/m}^2.\text{K}$
h_o	Heat Transfer Coefficient of Cooling water side, $\text{W/m}^2.\text{K}$
h_{fi}	Heat Transfer Coefficient of dirt (fouling) in broth side, $\text{W/m}^2.\text{K}$
h_{fo}	Heat Transfer Coefficient of dirt (fouling) in Cooling water side, $\text{W/m}^2.\text{K}$
C_p	Specific Heat Capacity, kJ/kg.K
ρ	Density, kg/m^3
M	Molecular Weight, kg/kgmol

Yield Coefficients

$$Y_{XS} = \frac{r_X}{-r_S} = \frac{\text{Amount of biomass produced in kg}}{\text{Amount of substrate consumed in kg}}$$

$$Y_{PX} = \frac{r_P}{r_X} = \frac{\text{Amount of product produced in kg}}{\text{Amount of biomass produced in kg}}$$

REFERENCES

- [1] Palaniraj, A., & Jayaraman, V. (2011). *Journal of Food Engineering*, 106(1), 1–12. doi:10.1016/j.jfoodeng.2011.03.035
- [2] Vignesh, P., Arumugam, A., & Ponnusami, V. (2015). *Bioprocess and Biosystems Engineering*, 38: 49-56. doi:10.1007/s00449-014-1242-1
- [3] Faria S, Vieira PA, Resende MM, Franca FP & Cardoso VL (2009). *Applied Biochemistry and Biotechnology*, 156:475–488. doi:10.1007/s12010-008-8485-8
- [4] Rushton J H, Costich E W & Everett H J (1950). *Chemical Engineering Progress*. 46:467-479.
- [5] Amanullah A, Satti S & Nienow A (1998) *Biotechnology Progress*, 14(2):265–269. doi:10.1021/bp9800079.

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- [6] Pinches, A, & Pallent, L. J. (1986). *Biotechnology and Bioengineering*, 28(10), 1484–96. doi:10.1002/bit.260281006.
- [7] Galindo, E. et. al. (1989). *Bioprocess Engineering*, 4, 113-118.
- [8] Hughmark GA., (1980). *Industrial & Engineering Chemistry Process Design and Dvelopment*. 19: 538-641
- [9] Amanullah, B., Tuttiett, B. & Nienow, A.W. (1998). *Biotechnology and Bioengineering*. 20;57(2):198-210.
- [10] Doran, P.M. (Published 1995). *Bioprocess Engineering Principles*. Elsevier Science & Technology Books. ISBN: 0122208552.
- [11] Sinnott, R.K. (4 ed. 2005). *Coulson and Richardson's Chemical Engineering Volume 6: Chemical Engineering Design*. Elsevier Science & Technology Books. ISBN 0 7506 65386.
- [12] Perry's Chemical Engineers' Handbook. 8th edition. The McGraw-Hill Companies, Inc. doi:10.1036/0071422943.