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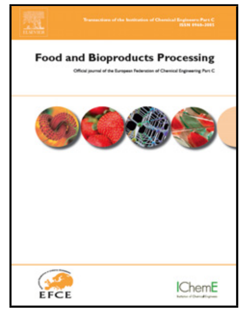

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Application of mathematical modelling for investigating oxygen transfer energy requirement and process design of an aerobic continuous stirred tank fermenter

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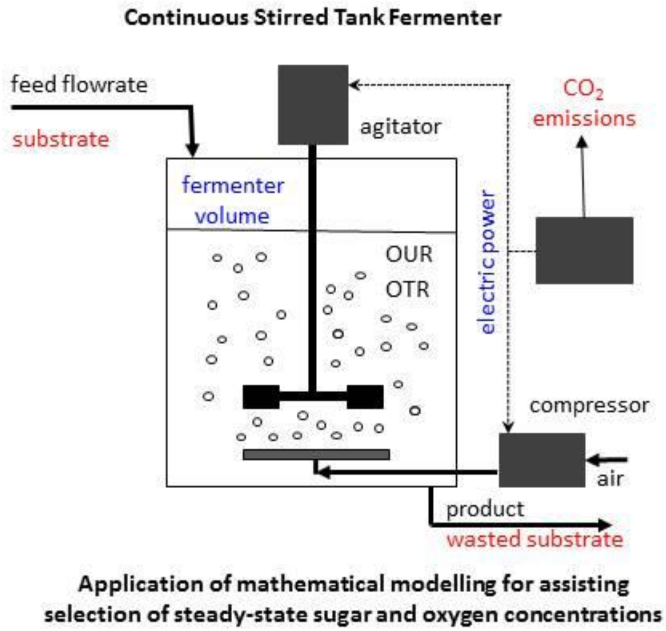
Graphical Abstract



Highlights

- Mathematical modelling can show conflicts between desired design outcomes in the process design of a continuous fermenter.
- Modelling can help select the values of steady-state sugar and oxygen concentrations for best compromise designs.
- Significant aeration system energy savings can be made by appropriate selection of operating variables.

ABSTRACT

Fermentation kinetic and oxygen transfer modelling coupled with energy analysis was applied to investigate how key input design variables influenced fermenter size, feed substrate requirement, wasted substrate and aeration system electrical energy requirement. The study showed that trade-offs and compromises are required to select the values of key input variables that can produce superior process designs in terms of the output variables. For example, reducing steady-state oxygen concentration reduced aeration system energy requirements and associated carbon footprint but increased fermenter size and associated cost. Mathematical modelling can assist in more precisely zoning in quantitatively on the selection of design input variable values that can produce a best compromise between conflicting design output variables. Mathematical modelling can also highlight design sensitivities. For example, if the steady-state sugar concentration is reduced below a certain value, then this can lead to an exponential increase in fermenter volume and associated cost, thus it is prudent to operate on the conservative side of this value.

Keywords: continuous stirred tank fermenter; process design; mathematical modelling; energy; environmental impact.

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List of symbols

A_T	cross-sectional area of fermenter (m^2)
C_{OG}	oxygen concentration in air bubble (mg L^{-1})
C_{OGI}	oxygen concentration in air entering fermenter (mg L^{-1})
C_{OGO}	oxygen concentration in air leaving fermenter (mg L^{-1})
C_{OL}	steady-state oxygen concentration in the fermentation broth (mg L^{-1})
D	impeller diameter (m)
D_R	dilution rate (h^{-1})
F	volumetric flowrate of feed entering fermenter (m^3 h^{-1})
F_G	inlet air volumetric flowrate (m^3 h^{-1})
F_{S0}	mass flowrate of sugar entering fermenter (kg h^{-1})
F_{SW}	mass flowrate of wasted sugar exiting fermenter (kg h^{-1})
k_La	volumetric oxygen mass transfer coefficient (h^{-1})
K_O	Monod kinetic constant for oxygen (g L^{-1})
K_S	Monod kinetic constant for sugar (g L^{-1})
M	Henry's Law constant
m_S	specific maintenance coefficient (h^{-1})
N	agitator rotational speed (s^{-1})
N_{PG}	agitator power number
OUR	oxygen uptake rate (g L^{-1} h^{-1})
OTR	oxygen transfer rate (g L^{-1} h^{-1})
Pag	agitator mechanical power input in gassed fermenter (kW)
P_{atm}	atmospheric pressure (Pa)
P_C	compressor mechanical power input (kW)
P_f	steady-state product concentration (g L^{-1})
P_i	atmospheric pressure + static head in fermenter (Pa)
P_R	mass flowrate of product exiting fermenter (kg h^{-1})
P_{tot}	sum of compressor and agitator electrical power inputs (kW)
S_f	steady-state sugar concentration (g L^{-1})
T	fermenter diameter (m)
V_L	fermenter working volume (m^{-3})

v_s	air superficial velocity (m h^{-1})
vvm	volume of air per minute per unit fermenter working volume (min^{-1})
X_f	steady-state cell concentration (g L^{-1})
Y_{XS}	Yield coefficient for biomass
Y_{PS}	Yield coefficient for product
α, β	fermentation model kinetic constants
δ, Φ	OUR model constants
μ	specific growth rate (h^{-1})
μ_{max}	maximum specific growth rate (h^{-1})
η_C, η_m	compressor isentropic efficiency, electric motor efficiency
γ	isentropic exponent of compression

1. Introduction

A continuous stirred tank fermenter (CSTF) operated at steady-state can be used to continuously produce fermentation products. Specification of key process design input variables, such as steady-state substrate concentrations, can be challenging, as there are usually many design objectives, such as minimising fermenter size, energy requirements and environmental impacts, that may conflict with each other. The environmental impacts are natural resource use, including feed substrate, and wastes / emissions, including wasted unutilised substrate and CO_2 emissions associated with energy provision to the CSTF. In this study, mathematical modelling is applied to the process design of a CSTF to investigate the determination of design input variables that can achieve satisfactory designs for producing a specific product production rate. The work considers the modelling of steady-state operation only so as to reduce the complexity of the analysis but it does recognise that non-steady-state operation, for example during CSTF start-up, will also influence overall system performance. An *Aspergillus niger* fermentation is modelled in this study, but the work is not about this particular fermentation; this is simply used as a case-study because there were data available in the literature that could be directly applied in the modelling.

In this study, oxygen transfer and its energy requirement are very important. In aerobic fermentations, oxygen is a critical substrate that needs continuous supply, as it can easily become rate-limiting due to its low solubility in water [1]. Steady-state oxygen concentration is a key input design variable for a CSTF as it influences this energy requirement but also influences fermentation kinetics which in-turn influences other variables, in particular fermenter volume and associated cost. The energy or power input associated with the aeration system consists of the compressor power requirement to supply an air flowrate and the agitator power requirement to improve mass transfer. Aeration system energy requirement is a significant cost in aerobic fermentations [2] and also contributes to the carbon footprint of fermentations. Reducing aeration system energy and associated costs and carbon footprint may be achieved through proper equipment selection, including careful selection of impeller type and impeller diameter to tank ratio [3]. Subsequently, energy minimisation can be achieved by optimal operation of air flowrate and agitator speed [2, 4-6].

Many studies have been conducted to show how agitation and aeration rate influence the oxygen transfer rate and in so doing influence cell growth and metabolite productivity [7-14]. The aeration system must transfer sufficient oxygen or the oxygen transfer rate (OTR) must be sufficient to meet the steady-state oxygen transfer rate (OUR) in a CSTF, so that oxygen does not adversely limit the fermentation kinetics which may result in a significantly larger fermenter volume than required. Oxygen transfer in a fermentation is strongly influenced by the hydrodynamic conditions, which are influenced by operating conditions, the physical chemical properties of the fermentation broth, geometrical parameters of the fermenter and the oxygen concentration in the broth [1, 15-17]. The main determinants of the mass transfer coefficient under direct operational control are the agitator mechanical power input per unit volume (P/V) and the air superficial velocity (v_s). Measurement and evaluation of the volumetric mass transfer coefficient (k_La) and how it is influenced by P/V and v_s is crucial in the design, operation and scale-up of fermentations [1, 11, 18-22]. Even though there is much work presented in the literature on oxygen transfer and fermentation dynamics there is not much presented on applying mathematical modelling to energy analysis of oxygen transfer in fermentations and how this interacts with other important process design output variables. Alves & Vasconcelos

[2] performed a mathematical optimisation procedure to minimise total power requirement subject to maintaining the oxygen concentration in the broth at a critical value, and showed power savings of 10 to 20% could be achieved by applying the optimisation procedure.

2. Mathematical modelling

The continuous stirred tank fermenter (CSTF) modelled has a six bladed Rushton turbine impeller used with a standard design configuration. The height to tank diameter ratio in stirred tank aerobic fermenters is typically two or greater [24] and the impeller diameter of turbine impellers is typically about one-third of the tank diameter, thus a height to tank diameter ratio of 2 and the impeller diameter to tank diameter ratio of 0.35 was used in this study. Details of the mathematical models are provided in the following sections and were implemented using Microsoft Excel.

2.1. Fermentation kinetics

Cell growth is modelled using a first order kinetic model in equation (1).

$$r_x = \mu X_f \tag{1}$$

where r_x is the cell growth rate, X_f is steady-state cell concentration and μ is the specific growth rate, which is modelled using the Monod model (equation 2)

$$\mu = \left(\frac{\mu_{max} S_f}{K_S + S_f}\right)\left(\frac{C_{OL}}{K_O + C_{OL}}\right) \tag{2}$$

where S_f and C_{OL} are the steady-state sugar and oxygen concentrations, respectively, μ_{max}, K_S and K_O are constants.

The rate of change of product concentration (r_p) and sugar concentration (r_s) due to microbial metabolism were modelled using the following equations 3 and 4.

$$r_p = \alpha\, r_x + \beta X_f \tag{3}$$

$$r_s = -\left(\frac{1}{Y_{XS}}\, r_x + \frac{1}{Y_{PS}}\, r_p + m_S X_f\right) \tag{4}$$

Values for the constants in the fermentation model equations were mainly obtained for an *Aspergillus niger* fermentation reported by Znad et al. [23], except for the values of Y_{XS}, Y_{PS} and m_S which were obtained from van’t Riet & Tramper [24]. These data are presented in Table 1. The *Aspergillus niger* fermentation [23] produced gluconic acid using glucose as the carbon substrate. Concentration values at the start of the fermentation were X_0 = 0.01g L^{-1}, S_0 = 150g L^{-1} and P_0 = 0 g L^{-1}, and the fermentation was completed when S_f was reduced to 0.1 g L^{-1}.

Steady-state sugar and product mass balance equations are provided in equations (5) and (6).

$$r_s = -D_R(S_0 - S_f) \qquad (5)$$

$$r_p = D_R(P_f - P_0) \qquad (6)$$

where D_R is the dilution rate and P_f is the steady-state product concentration.

The product yield is defined in equation (7).

$$Product\ Yield = \frac{P_f - P_0}{S_0 - S_f} \qquad (7)$$

2.2. Fermenter working volume and substrate utilisation

The steady-state product production rate (P_R) by the CSTF is specified as 100 kg h^{-1}. P_R is also given by equation (8).

$$P_R = F\ P_f \qquad (8)$$

where F is the feed volumetric flowrate.

For a CSTF operating at steady-state, equation (9) applies.

$$\mu = D_R = \frac{F}{V_L} \qquad (9)$$

where D_R is the dilution rate and V_L is the working volume of the CSTF. Equations (8) and (9) were used to calculate F and V_L.

The mass flowrate of sugar substrate entering the CSTF (F_{S0}) is given in equation (10)

$$F_{S0} = F\ S_0 \qquad (10)$$

The mass flowrate of wasted sugar leaving the CSTF (F_{SW}) is given in equation (11)

$$F_{SW} = F\ S_f \qquad (11)$$

2.3. Oxygen transfer

The oxygen uptake rate (OUR) was modelled using equation 12.

$$\mathrm{OUR} = \delta \frac{\mathrm{dX}}{\mathrm{dt}} + \phi \, \mathrm{X} \qquad (12)$$

where δ = 0.27824 and Φ = 0.00487 h^{-1} [23].

The mass transfer equation (13) was used to calculate the k_La value required to supply the oxygen transfer rate (OTR) to satisfy the OUR at steady-state:

$$OTR = k_L a (C_{OL}^* - C_{OL}) \qquad (13)$$

where

$$C_{OL}^* = \frac{C_{OG}}{M} \qquad (14)$$

C_{OG} is the oxygen concentration in the air bubbles and M is the Henry's law equilibrium constant (= 35). C_{OG} varies from the concentration of oxygen in the ambient air (C_{OGI} = 280 mg L^{-1}) to the concentration of oxygen in the air leaving the fermenter (C_{OGO}). Thus equation (15) was used to evaluate an average equilibrium concentration of oxygen in the liquid.

$$C_{OL}^* = \frac{(C_{OGI} + C_{OGO})/2}{M} \qquad (15)$$

A mass balance on the fermenter was used to evaluate another expression for OTR (equation 16).

$$OTR = \frac{F_G}{V_L} (C_{OGI} - C_{OGO}) \qquad (16)$$

where F_G is air volumetric flowrate and V_L is the working volume of the fermenter.

The correlation relationship between k_La and agitator mechanical power input in the gassed fermenter (Pag) and air superficial velocity (v_s) is given by equation 17. This equation was used to calculate Pag in the mathematical simulations.

$$k_L a = K \left(\frac{Pag}{V_L}\right)^{n1} (v_s)^{n2} \qquad (17)$$

The values of the constants were K = 0.026, n_1 = 0.4 and n_2 = 0.5 and these were obtained from van't Riet [25]. Equation 17 is an important correlation and the values of the constants in this equation should be experimentally evaluated in the application of this modelling approach to a real fermentation. Furthermore, the size of the fermenter volume may influence the values of constants in equation 17. Even though the fermenter volume changes in this study, a simplifying assumption is made that the values of the constants do not vary in equation 17. However, in the application of the mathematical approach to a real fermentation, some work should also be undertaken to investigate how scale-up influences these constants.

The air superficial velocity (v_s) is defined in equation 18.

$$v_s = \frac{F_G}{A_T} \tag{18}$$

where A_T is the cross-sectional area of the fermenter. The parameter vvm is commonly used instead of v_s and this is defined in equation 19.

$$vvm = \frac{F_G}{V_L} \tag{19}$$

where the units are expressed as minutes^{-1}.

2.4. Flooding and phase equilibrium constraints

The superficial air velocity is limited by impeller flooding and this depends on the mechanical power input. The correlation in equation 20 was obtained using information obtained from Benz [26] for a 6-bladed turbine impeller and was used to evaluate the air volumetric flowrate at the onset of flooding (F_{GF}).

$$\left(\frac{F_{GF}}{ND^3}\right) = 30\left(\frac{N^2 D}{g}\right)\left(\frac{D}{T}\right)^{3.5} \tag{20}$$

where D and T are impeller and tank diameters, respectively. The impeller rotational speed (N) was evaluated from the power number equation (21).

$$Pag = N_{PG}\rho N^3 D^5 \tag{21}$$

where the density (ρ) = 1 kg L^{-3} and N_{PG} is the impeller power number.

The 2 equations (20 and 21) can be used to formulate equation 22.

$$F_{GF} = \left(\frac{30}{gDN_{PG}\rho}\right) Pag \left(\frac{D}{T}\right)^{3.5} \tag{22}$$

This shows that F_{GF} is directly proportional to Pag and inversely proportional to N_{PG}. A constant power number of 6 was used in study [24]. Even though the power number will decrease with greater aeration, this constant value acts a conservative or lower estimation of the flooding air flowrate.

The oxygen concentration in the air leaving the fermenter (C_{OGO}) was limited by the equilibrium constraint (23).

$$C_{OGO} \geq M(C_{OL}) \qquad (23)$$

2.5. Aeration system energy requirement

The agitator mechanical power input requirement was estimated from equation (17). The compressor mechanical power requirement for a specific air flowrate was estimated from equation 24 [17].

$$P_C = \frac{\gamma}{\gamma - 1} F_G P_{atm} \left(\left(\frac{P_i}{P_{atm}} \right)^{\frac{\gamma-1}{\gamma}} - 1 \right) \left(\frac{1}{\eta_C} \right) \qquad (24)$$

where P_{atm} is atmospheric pressure and Pi is the atmospheric pressure plus the static pressure acting on the bottom of the fermenter due to weight of liquid, $\gamma = 1.4$. η_C is the isentropic efficiency of the compressor (assumed to be constant at 0.7). The sum of the agitator and compressor electrical power requirements (P_{tot}) was given by equation 25.

$$P_{tot} = \left(\frac{Pag + P_C}{\eta_m} \right) \qquad (25)$$

where η_m is the electric motor efficiency (assumed to be constant at 0.9 for both the agitator and compressor).

3. Results and discussion

3.1 Fermentation kinetics, fermenter volume and feed / wasted sugar substrate

3.1.1 Fermentation kinetics

The fermentation kinetics as influenced by the steady-state sugar concentration (S_f) (at a steady-state oxygen concentration of 2 mg L^{-1}) is shown in Fig. 1. Fig. 1a shows the microbial cell growth. The specific growth rate decreases continuously from 0.27 h^{-1} at S_f = 120 g L^{-1} to 0.015 h^{-1} at S_f = 1 g L^{-1}, noting that these values are well below the maximum specific growth rate of 0.668 h^{-1}. The cell growth rate is mainly controlled by the sugar concentration when the oxygen concentration is 2 mg L^{-1}, as highlighted later in Fig. 3.

The cell growth is complex with steady-state cell concentration (X_f) reaching a maximum of about 19 g L^{-1} at S_f = 20 g L^{-1}. The steady-state product concentration (P_f), product yield, rate of change of product concentration (r_p) and sugar concentration (r_s) due to microbial metabolism are presented in Fig. 1b. As expected, P_f decreases with increased S_f, however there are variations in the product yield ranging from about 64% at S_f = 120 g L^{-1} and 81% at S_f = 1 g L^{-1}. The values for r_p and r_x both display a maximum and r_s displays a minimum.

3.1.2 Fermenter volume and feed / wasted sugar substrate

In the process design of a CSTF to produce a specified rate of product leaving the fermenter, S_f is a key variable to specify, as it influences fermenter volume requirement, feed sugar requirement and wasted sugar leaving the fermenter. Broad trends can be expected, however good fermentation kinetic models coupled with mass balances can help provide a more precise quantitative description that can help in selecting S_f. Fig. 2 shows the effect of S_f. In Fig. 2a, increasing S_f results in both higher feed sugar requirement and higher wasted sugar leaving the fermenter. This is to be expected as higher S_f means more sugar will be wasted and consequently more feed sugar is required to meet the product production specification.

In Fig 2b, increasing S_f results in higher feed flowrate, which is to be expected as more feed sugar is required, however it is not a linear relationship due to the complex non-linear fermentation kinetics. The fermenter working volume is a key design variable. The behavior is somewhat complex, showing a minimum volume at S_f = 50 g L^{-1}. The working volume (V_L) is determined from equation (9) and re-arranging it gives equation (26).

$$V_L = \frac{\mathrm{F}}{D_R} = \frac{\mathrm{F}}{\mu} \qquad (26)$$

From this equation, it can be seen that there is a trade-off between F and μ, because they both decrease as S_f decreases and thus trade-off against each other in the determination of the working volume, which produces the minimum.

Considering the above and the specification of S_f from a process design perspective, it would be desirable to select a value of S_f that could minimize working volume, feed sugar requirement and wasted sugar. From Fig. 2, there is a trade-off or process optimization to be made. This will be considered later in section 3.4 together with the impact of S_f on the energy requirements for oxygen transfer, which is investigated in the next section.

3.2 Electrical power requirement for oxygen transfer

The steady-state oxygen concentration in the fermenter liquid (C_{OL}) will influence cell growth and the oxygen mass transfer driver, which in turn will influence the oxygen transfer rate and the electrical power requirement. The Monod model for oxygen as the rate-limiting substrate in the presence of abundant sugar is presented in Fig. 3 over the relevant C_{OL} range of interest. This shows that at C_{OL} = 8 mg L^{-1} the specific growth rate is near the maximum and only slowly decreases as C_{OL} is reduced to about 2 mg L^{-1}, after which there is a much more precipitous fall. As a result of this, in the initial part of the power requirement analysis a C_{OL} value of 2 mg L^{-1} was initially investigated, and the effect of varying C_{OL} is considered later.

3.2.1 Effect of vvm and steady-state sugar substrate concentration

To control C_{OL} at 2 mg L^{-1}, the oxygen transfer system must be able to supply an OTR equal to the OUR. This is implemented by a combination of air flow and mechanical agitation, subject to the constraints of agitator flooding and phase equilibrium outlined in section 2.4. The OTR and power requirements of the compressor and agitator will depend on the OUR. Fig. 4 shows how S_f influences OUR. The OUR shows a maximum value, however the fermenter volume varies with S_f, thus Fig. 4 also shows the total oxygen uptake rate in the fermenter volume, which shows a gradual reduction from S_f = 120 to 20 g L^{-1} before reducing more significantly at lower values of S_f. Simulations were performed to evaluate the effect of vvm on the power requirement of the compressor and agitator at different values of S_f. Some of these data are presented in Fig. 5 for two values of S_f. The vvm values in Fig. 5a and 5 are considerably different but this is due to the different OUR requirements as these depend on S_f, as illustrated in Fig. 4.

As expected, Fig. 5 shows that the compressor power increases as vvm increases and there is a corresponding decrease in agitator power to supply the OTR required to meet the OUR. However, compressor power increases linearly with vvm while agitator power decreases in an exponential fashion. The trade-off between compressor and agitator power results in a value of vvm that minimises total power. In the simulations, this minimum tended to be located at a value of vvm that is beyond the flooding value. Consequently, the minimum total power that also satisfies the constraints was located at the on-set of flooding. Fig. 5 also shows that there is a significant “plateau” before flooding where the total power is not changing much. It also shows that care needs to be taken in the selection of vvm, so as to avoid excessive total power requirement, due to excessive agitator power in particular, and to remain within constraints, especially the flooding constraint. Consequently, major savings in aeration system energy requirement can be made by careful selection of vvm and agitator power input requirement, and mathematical modelling can assist in this selection.

3.2.2 Agitator and compressor power optimisation

From the above section, there are design values of vvm (and corresponding air compressor power) and agitator power that will minimise total electrical power requirement to supply the OTR for an OUR at a given S_f. These were evaluated as a functions of S_f for C_{OL} = 2 mg L^{-1}, and these data are presented in Fig. 6. These data show that total power is nearly flat at around 7 kW in the range of S_f = 50 to 120 g L^{-1}. At lower S_f values, power values decrease, especially below S_f = 20 mg L^{-1}. This is most likely due to the decrease in the total oxygen uptake rate in fermenter volume (OUR*V_L) illustrated in Fig. 4. Overall, Fig. 6 shows that is desirable to operate at lower S_f values from the perspective of electrical power requirement for oxygen transfer.

3.3 Effect of steady-state oxygen concentration (C_{OL})

C_{OL} will influence fermentation kinetics, which in-turn can influence fermenter volume, feed flowrate, feed and wasted sugar substrate. It will also influence the electrical power requirement for the aeration system, because lowering C_{OL} will increase the oxygen mass transfer driving force which will reduce the k_La required to supply a required OTR. Consequently, this section investigates the influence of C_{OL} on these aspects.

3.3.1 Fermenter volume, feed flowrate and feed/wasted sugar substrate

As presented and discussed earlier in section 3.2, Fig.3 shows the influence of C_{OL} on specific growth rate, thus C_{OL} would be expected to have significant impacts at lower values of around 1 mg L^{-1} and less. Simulations, like those in section 3.2, were run at C_{OL} values ranging from 0.1 to 6 mg L^{-1}, and the results are presented in Fig. 7. Fig. 7a shows the effect of C_{OL} on wasted sugar. There are minor differences but these appear to be very small. Similar trends were obtained for the feed volumetric flowrate and feed sugar requirement. Overall, it can be concluded that varying C_{OL} has very little impact on these variables.

The influence of C_{OL} on the fermenter working volume is presented in Fig. 7b. This shows a major influence, especially at low concentrations, e.g. at less than 0.5 mg L^{-1}. Reducing C_{OL} reduces specific growth rate and considering equation (26), this results in an increase in fermenter volume as the feed flowrate is not much affected. Consequently, the effect of C_{OL} on fermenter volume is directly related to the effect of C_{OL} on the specific growth rate.

3.3.3 Power requirement for oxygen transfer and trade-off with fermenter volume

Fig. 8 shows the influence of C_{OL} on the total minimum electrical power requirement at each S_f. Each line is for a constant C_{OL} value and each point represents the minimum total electrical power requirement at the specified S_f, as highlighted in section 3.2. As expected, reducing C_{OL} reduces the power requirement because this increases the oxygen mass transfer driver which reduces the k_La required.

Considering section 3.3.1, there is now an obvious trade-off in terms of specifying a value for C_{OL}. On one hand, reducing C_{OL} reduces electrical power requirement but on the other hand it increases fermenter working volume. Table 2 presents some calculations on the impact of C_{OL} on the percentage change in volume and power in comparison to values for C_{OL} = 2 mg L^{-1}. For example, reducing C_{OL} from 2 to 1 mg L^{-1} results in a 14% increase in fermenter volume and a 20% reduction in total electrical power.

3.4 Process design optimisation and trade-offs

From a process design perspective, the selection of S_f and C_{OL} are very important. However as highlighted in this work, there are no values for these variables that are totally desirable because there are conflicts between the desired objectives of minimising the following:

- Fermenter volume
- Feed flowrate and sugar substrate requirement
- Wasted sugar substrate
- Electric power requirement for oxygen transfer
- Greenhouse gas emissions associated with electric power supply
- Cost

For a given C_{OL}, reducing S_f had beneficial impacts in reducing feed flowrate, sugar requirement and wasted sugar. It also reduces electric power requirement for oxygen transfer. However, the fermenter volume showed a minimum value, and when S_f was reduced below about 20 g L^{-1} the volume started to exponentially increase. Reducing C_{OL} reduced electrical power requirement, however this tended to increase fermenter volume, especially at lower C_{OL} values below 1 mg L^{-1}, where the volume tended to increase exponentially. Consequently, there are no values of S_f and C_{OL} that will minimise all the desired objectives and thus trade-offs must be considered to zone in on satisfactory values. Considering the results of the simulations may help in zoning in on suitable values. For, example, selecting a C_{OL} value of 2 mg L^{-1} and an S_f value of 20 g L^{-1}. C_{OL} = 2 mg L^{-1} appears to represent a good trade-off between electrical power requirement and fermenter size, while S_f = 20 g L^{-1} is possibly as low as can be achieved without exponential increase in the size of the fermenter. A more structured optimisation approach that is commonly used would be to evaluate values of S_f and C_{OL} that minimise financial cost subject to constraints (such as limits on environmental emissions).

3.5 Effect of k_La correlation power requirement for oxygen transfer

The k_La correlation is a critical model equation for the determination of power requirements. It is influenced by many parameters, including agitator type, vessel geometry and position of agitator in the vessel, and the physical properties of the fermentation broth, such as viscosity and bubble coalescence. Benz [22] selected three k_La correlations commonly used from the literature along with two from his own industrial practice and compared their impact on compressor, agitator and total energy requirements in a batch vessel. In this section, CSTF simulations were performed for each of these five correlations. These simulations were carried to investigate the influence of the k_La correlation on total minimum electrical power requirement (at C_{OL} = 2 mg L^{-1}). The correlation constants are presented in Table 3 and the results of the simulations are presented in Fig. 9. There is significant variation in power requirements depending on the correlation used. The highest power requirement correlation had power requirements of over double the lowest power requirement correlation.

4. Conclusions

Mathematical modelling can be usefully applied in the process design and optimisation of a CSTF. Steady-state sugar concentration (S_f) and oxygen concentration (C_{OL}) are two important input process design variables that influence key output variables, such as fermenter size, energy requirements and environmental impact. Reducing S_f had beneficial effects in terms of reducing feed and wasted sugar substrate and their associated environmental impacts, however below a certain value this leads to an exponential increase in fermenter volume and associated cost. Reducing C_{OL} reduced aeration system energy requirements and associated carbon footprint but impacted on fermentation kinetics and increased fermenter size and associated cost. This shows that varying S_f and C_{OL} may be beneficial for some design output variables but conflict with or be detrimental to the values of others, thus trade-offs and compromises are required to determine superior process designs. Mathematical modelling can assist in more precisely zoning in quantitatively on the selection of values of S_f and C_{OL} that can produce a best compromise between conflicting design output variables. It can also highlight design sensitivities in the sense that if S_f or C_{OL} is reduced below or increased above a certain value, then some design output variables may change very rapidly in an adverse manner, such as reducing S_f below a certain value leading to an exponential increase in fermenter volume and associated cost. Selection and control of air flowrate and agitator power requirement has a major influence on the total energy requirement of the aeration system, thus careful selection can result in much lower energy requirements while remaining within system constraints. Finally like in any other application of mathematical modelling, it is critical that the model equations, including values of constants, are good and representative, in particular the fermentation kinetics, OUR equation and k_La correlation. This typically requires extensive practical work to achieve.

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FIGURES

Fig. 1. Relationship between steady-state sugar concentration and (a) cell growth and (b) product concentration (Pf), yield, rate of product formation (rp) and substrate utilization rate (rs). [steady-state oxygen concentration is 2 mg L^{-1}]

Fig. 2. Relationship between steady-state sugar concentration and (a) feed substrate requirement and wasted substrate, and (b) feed flowrate and fermenter working volume. [steady-state oxygen concentration is 2 mg L^{-1}]

Fig. 3. Effect of steady-state oxygen concentration on specific growth rate in the presence of abundant sugar.

Fig. 4. Effect of steady-state sugar concentration on oxygen uptake rate (OUR) and total oxygen uptake rate in the fermenter volume ($OUR*V_L$). [steady-state oxygen concentration is 2 mg L^{-1}]

Fig. 5. Effect of vvm on compressor, agitator and total electrical power requirements: steady-state sugar concentration (a) 80 g L^{-1}, (b) 5 g L^{-1} [steady-state oxygen concentration is 2 mg L^{-1}]

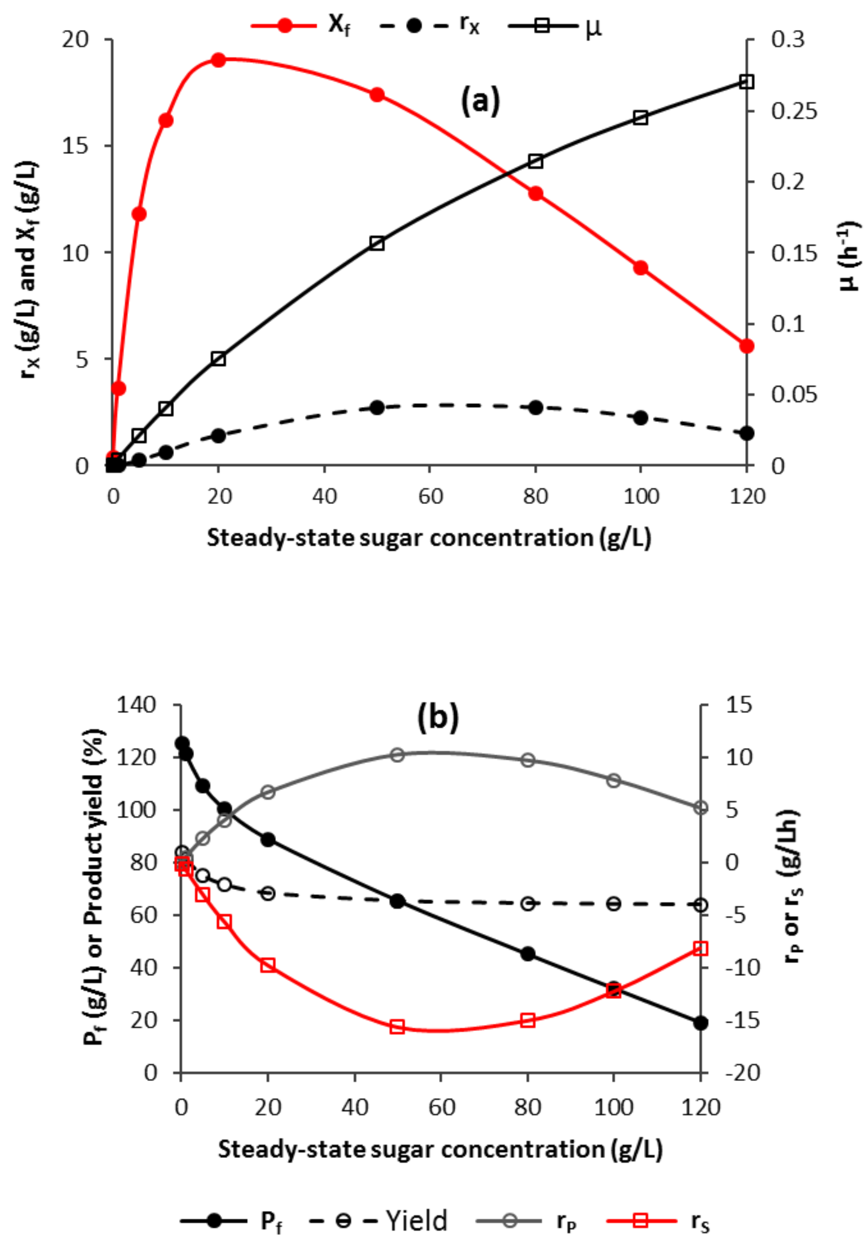
Fig. 6. Minimum total electrical power required (and corresponding compressor and agitator power requirements) at each steady-state sugar concentration value. [steady-state oxygen concentration is 2 mg L^{-1}]

Fig. 7. Effect of steady-state oxygen concentration on (a) wasted substrate and (b) fermenter working volume.

Fig. 8. Influence of steady-state oxygen concentration on minimum total electrical power requirement.

Fig. 9. Influence of k_La correlation (Table 3) on minimum total electrical power requirement.
[steady-state oxygen concentration is 2 mg L^{-1}]

Figure 1



X_f
r_X
μ
(a)
r_X (g/L) and X_f (g/L)
μ (h^{-1})
Steady-state sugar concentration (g/L)
(b)
P_f (g/L) or Product yield (%)
r_P or r_S (g/Lh)
Steady-state sugar concentration (g/L)
P_f
Yield
r_P
r_S

Figure 2

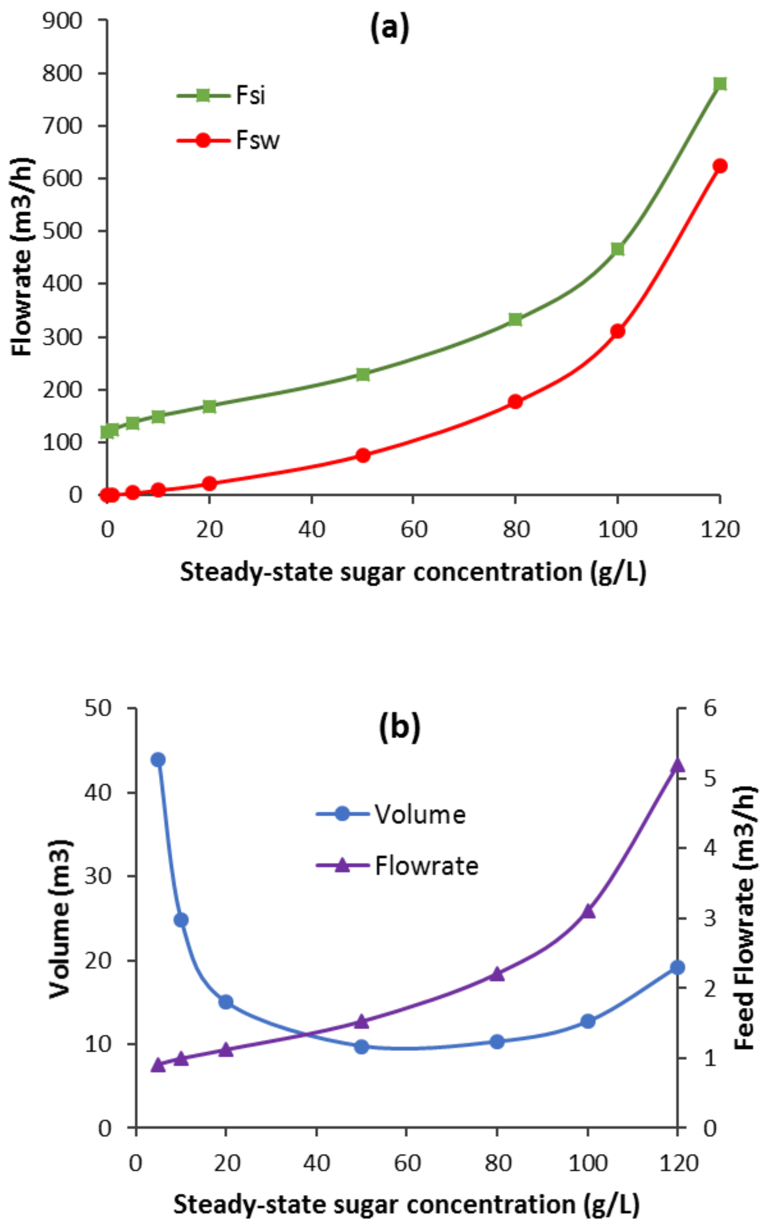

(a)
Fsi
Fsw
Flowrate (m3/h)
Steady-state sugar concentration (g/L)
(b)
Volume
Flowrate
Volume (m3)
Feed Flowrate (m3/h)
Steady-state sugar concentration (g/L)

Figure 3

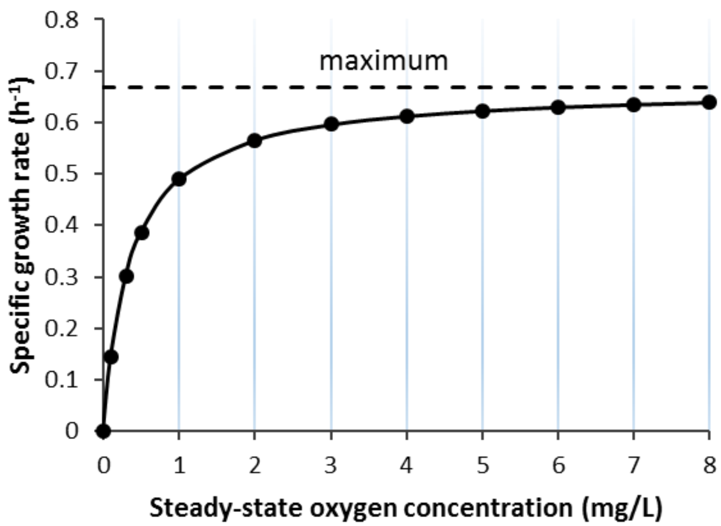
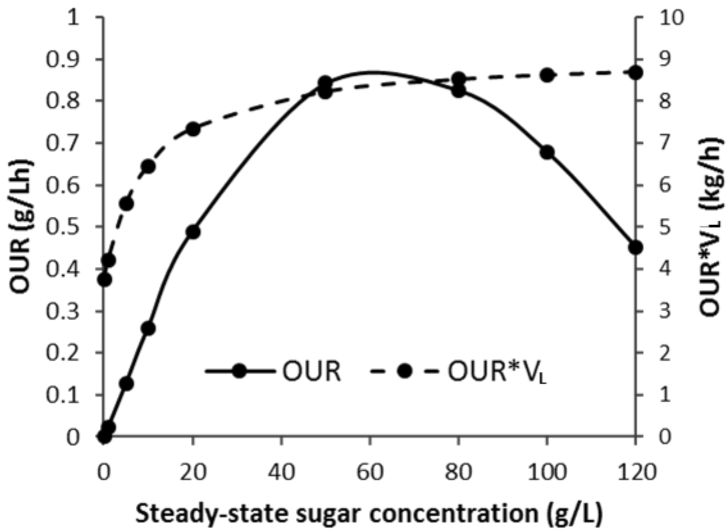

maximum
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
1
2
3
4
5
6
7
8
Specific growth rate (h-1)
Steady-state oxygen concentration (mg/L)

Figure 4



OUR (g/Lh)
OUR*V$_L$ (kg/h)
Steady-state sugar concentration (g/L)
OUR
OUR*V$_L$
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
0
1
2
3
4
5
6
7
8
9
10
0
20
40
60
80
100
120

Figure 5

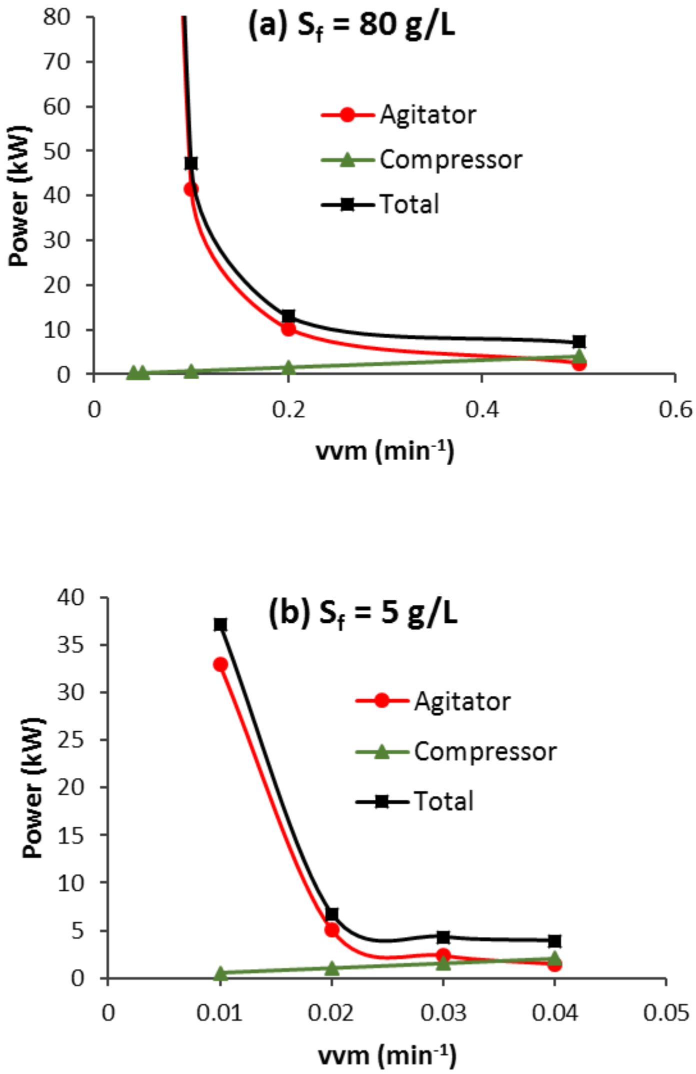

(a) S_f = 80 g/L
Agitator
Compressor
Total
Power (kW)
vvm (min^{-1})
0
10
20
30
40
50
60
70
80
0
0.2
0.4
0.6
(b) S_f = 5 g/L
Agitator
Compressor
Total
Power (kW)
vvm (min^{-1})
0
5
10
15
20
25
30
35
40
0
0.01
0.02
0.03
0.04
0.05

Figure 6

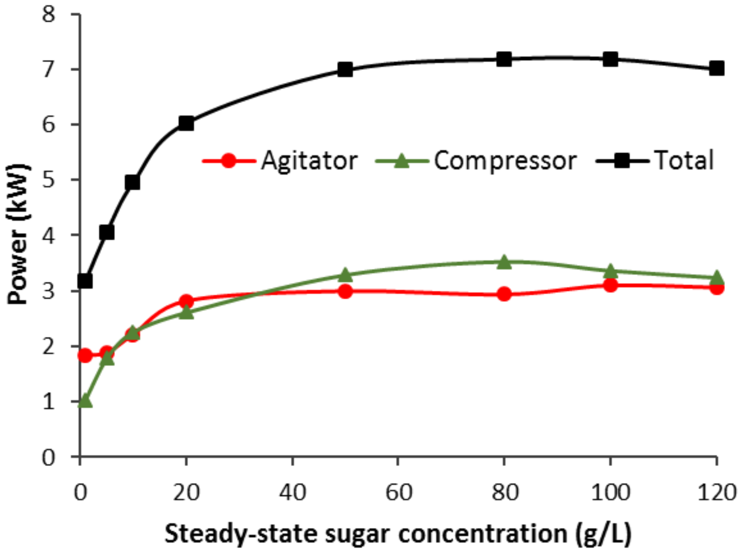

Power (kW)
0
1
2
3
4
5
6
7
8
0
20
40
60
80
100
120
Steady-state sugar concentration (g/L)
Agitator
Compressor
Total

Figure 7

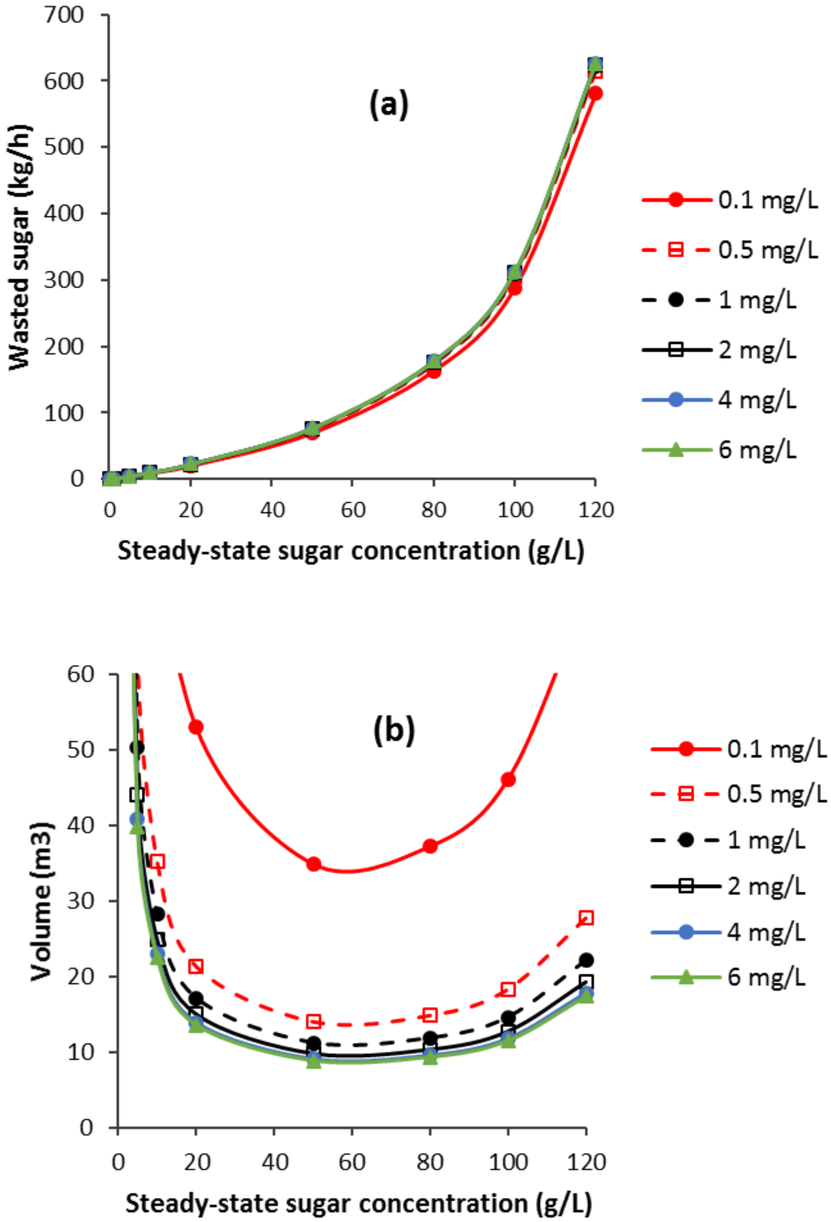
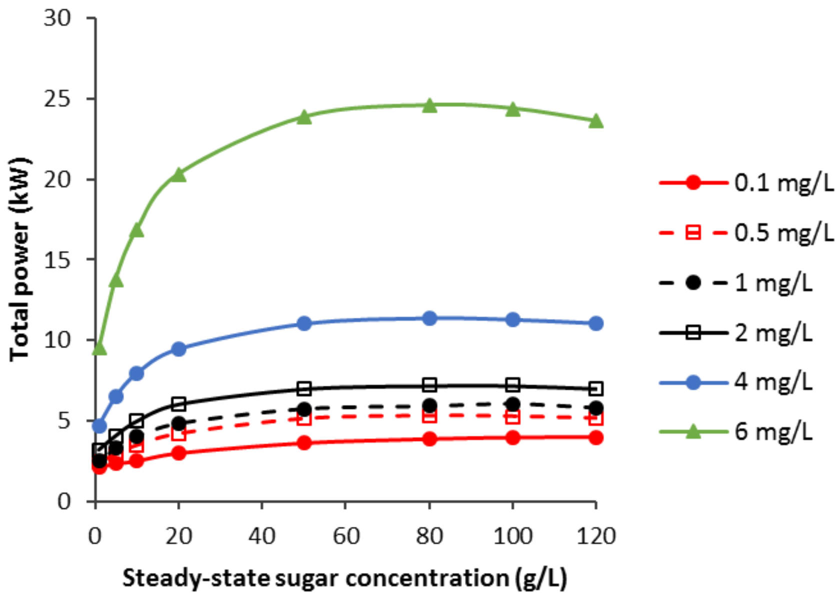
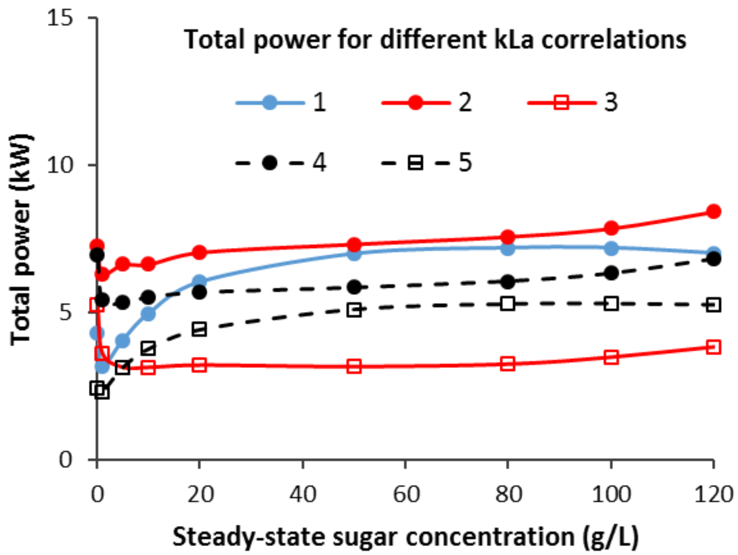

(a)
Wasted sugar (kg/h)
Steady-state sugar concentration (g/L)
0.1 mg/L
0.5 mg/L
1 mg/L
2 mg/L
4 mg/L
6 mg/L
(b)
Volume (m3)
Steady-state sugar concentration (g/L)
0.1 mg/L
0.5 mg/L
1 mg/L
2 mg/L
4 mg/L
6 mg/L

Figure 8



30
25
20
15
10
5
0
Total power (kW)
0
20
40
60
80
100
120
Steady-state sugar concentration (g/L)
0.1 mg/L
0.5 mg/L
1 mg/L
2 mg/L
4 mg/L
6 mg/L

Figure 9


Total power for different kLa correlations
1
2
3
4
5
Total power (kW)
0
5
10
15
0
20
40
60
80
100
120
Steady-state sugar concentration (g/L)

TABLES

Table 1. Values for constants in fermentation kinetic model

μ_{max} (h^{-1})	K_S (g L^{-1})	K_O (g L^{-1})	α	β (h^{-1})	Y_{XS}	Y_{PS}	m_S (h^{-1})
0.668	130.902	0.000363	2.9220	0.1314	0.55	1	0.025

Table 2. Effect of steady-state oxygen concentration (C_{OL}) on the percentage change in the fermenter working volume and minimum total electrical power requirement in comparison to corresponding values at C_{OL} = 2 mg L^{-1}. [Steady-state sugar concentration = 20 g L^{-1}]

C_{OL} (mg L^{-1})	% change in working volume	% change in electrical power
6	-9	237
4	-7	57
2	0	0
1	14	-20
0.5	42	-30
0.1	254	-50

Table 3. Values of constants in k_La correlations.

k_La correlations and references	Constants K	n1	n2
1. Bakker [27]	0.015	0.6	0.6
2. van't Riet non-coalesce [25]	0.026	0.4	0.5
3. van't Riet coalesce [25]	0.002	0.7	0.2
4. Benz broth 1 [22]	0.015	0.55	0.6
5. Benz broth 2 [22]	0.088	0.542	0.741