

Project 5: Complex systems

24.05.2024

Submission Deadline: **Thursday, 6th of June**, at 23:59h.

Submission Format: Single PDF file.

Page Limit: **Maximum of 9 pages** per group.

Submission Platform: Upload to Moodle.

This project consists of 3 exercises.

In this report, we expect that you:

- (i) Report the numerical answers and plots obtained to define the correct units!
- (ii) Briefly explain how you obtained these answers.
- (iii) Give an interpretation of the values/plots obtained.

You can use the template file found in Moodle.

Alongside your report, you must upload all related code files. This includes MATLAB files (either .m files or MATLAB notebook .mlx files) or Python files (.py files or Jupyter notebook files). The code should run by executing the script/main function **without extra arguments or external data**.

Organise your code files logically, dividing them into sections. Each section should be well-**documented with comments** to explain the code and the steps involved in your procedure.

Remarks

1. As a general consensus we define that a process becomes oxygen limited when at any stage of this process $C_L \leq 3K_{CL}$, where C_L is the amount of the dissolved oxygen in the liquid phase and K_{CL} the saturation constant of the dissolved oxygen.
2. For all questions, solve the ODE systems until steady state is reached.

EXERCISE 1

The influence of gassing rate and stirrer speed on an enzymatic, aerated reactor (Figure 1) is investigated. The outlet gas is assumed to be essentially air, which eliminates the need for a gas balance for the well-mixed gas phase.

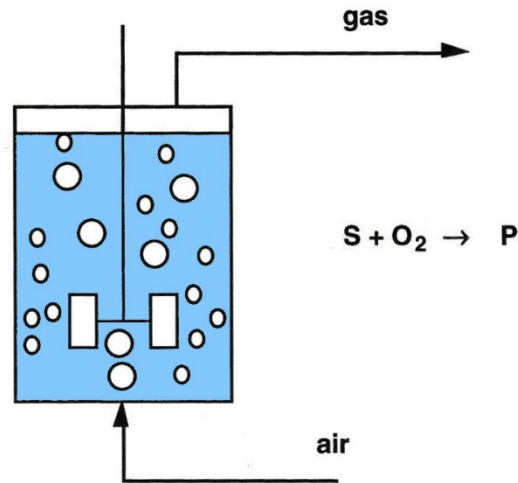


Figure 1: Schema of the enzymatic oxidation batch reactor

The reaction kinetics are described by a double hyperbolic relation:

$$r_S = V_m \frac{S}{K_S + S} \frac{C_L}{K_{CL} + C_L}$$

,where C_L is the concentration of dissolved oxygen.

The batch mass balances lead to the equations:

$$\begin{aligned} \frac{dS}{dt} &= -r_S \\ \frac{dC_L}{dt} &= k_L a (C_L^* - C_L) - Y_{O/S} \cdot r_S \\ \frac{dP}{dt} &= Y_{P/S} \cdot r_S \end{aligned}$$

The transfer coefficient, $k_L a$, varies with the stirring rate (N) and aeration rate (G) according to:

$$k_L a = k \cdot N^3 \cdot \sqrt{G}$$

The reactor is set up with 100 gL⁻¹ of substrate and negligible amount of product. We consider that there is about 6 mgL⁻¹ gas solved in the liquid of the reactor.

Further consider following parameters:

Oxygen transfer: $k = 3.2 \times 10^{-13} \text{ m}^{-\frac{3}{2}} \text{ h}^{\frac{5}{2}}$, $N = 30,000.0 \text{ h}^{-1}$, $C_L^* = 6 \text{ mg L}^{-1}$

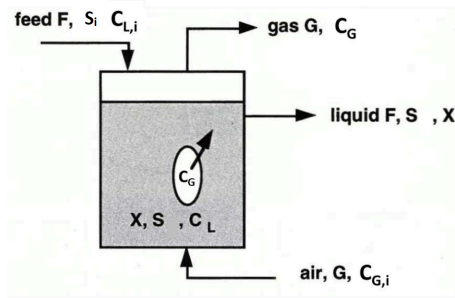
Enzyme kinetics: $V_m = 16 \text{ g L}^{-1} \text{ h}^{-1}$, $K_S = 7 \text{ g L}^{-1}$, $K_{CL} = 0.3 \text{ mg L}^{-1}$

Yield: $Y_{O/S} = 5 \text{ mg/g}$, $Y_{P/S} = 1.5 \text{ g/g}$

- a) Simulate the model with the parameters given above and assume an aeration rate of $G = 30 \text{ m}^3 \text{ h}^{-1}$. Verify that your system is not oxygen limited. Document your findings using a proper plot of systems concentrations.
- b) Find the aeration rate at which the reaction becomes oxygen limited. Plot therefore the minimum dissolved oxygen concentration as a function of the aeration rate.
- c) Set the aeration rate to the value found in b) and reduce the maximum substrate consumption rate V_m by half. Does the average product formation rate (from $t=0$ till the beginning of the steady state) decrease by $\frac{1}{2}$? (perform analysis for $V_m = V_m$ and $V_m = V_m/2$) Is the reaction still oxygen limited?
- d) For the 2 values of V_m in c) plot and discuss the time evolution of the dissolved oxygen concentration
- e) In the oxygen-limited conditions as found in b), decrease N by 15% and comment the change of $k_L a$, C_L and r_s . Consider the original value of V_m
- f) Find 5 combinations of N and G so that you achieve non-oxygen limiting conditions, justify your choices. Plot the variation in the product formation curves for each case. Discuss the effect of N and G on product formation.

EXERCISE 2

In an aerated continuous fermenter, cell growth is limited by the oxygen mass transfer rate, and hence by the dissolved oxygen concentration. It is also inhibited by an **inhibitory substrate S**. Liquid phase balances for X , S and O_2 in the liquid phase are therefore used, together with a gas phase oxygen balance to determine the rate of O_2 supply. To avoid washout of cells, it is important that the reactor should never enter the range of inhibitory behavior. A schematic representation of a continuous aerated fermenter is given in the figure below.



The mass balances are as follows:

$$\frac{dX}{dt} = -\frac{F}{V_L}X + \mu X$$

$$\frac{dS}{dt} = \frac{F}{V_L}(S_i - S) - \frac{1}{Y_{X/S}}\mu X$$

$$\frac{dC_L}{dt} = \frac{F}{V_L}(C_{Li} - C_L) - \frac{Y_{O/S}}{Y_{X/S}}\mu X + K_L a (C_L^* - C_L)$$

$$\frac{dC_G}{dt} = \frac{G}{V_G}(C_{Gi} - C_G) - K_L a \frac{V_L}{V_G}(C_L^* - C_L)$$

With the growth rate:

$$\mu = \frac{\mu_m S}{K_S + S + \frac{S^2}{K_I}} \cdot \frac{C_L}{K_{C_L} + C_L}$$

The oxygen equilibrium relates the concentration in the gas phase to the liquid phase saturation concentration,

$$C_L^* = M \cdot C_G$$

The gas holdup fraction is

$$V_G = \varepsilon \cdot V_L$$

The Oxygen Uptake Rate is the mass of oxygen that is consumed in the reaction per unit time (uptaken by the cells):

$$OUR = \frac{Y_{O/S}}{Y_{X/S}} \cdot \mu \cdot X \cdot V_L$$

Parameter values:

$$\begin{aligned}\mu_m &= 0.9 h^{-1} \\ K_s &= 0.21 g/L \\ K_I &= 1.5 g/L \\ Y_{X/S} &= 0.6 \\ K_{CL} &= 0.2 mg/L \\ Y_{O/S} &= 160 mg/g \\ K_L a &= 70 h^{-1} \\ M &= 0.0314 \\ F &= 6.5 L/h \\ V_L &= 90 L \\ G &= 5000 L/h \\ \varepsilon &= 0.2 \\ C_{Li} &= 6 mg/L \\ C_{Gi} &= 250 mg/L \\ S_i &= 30 g/L\end{aligned}$$

Initial conditions:

$$\begin{aligned}X(0) &= 1 g/L \\ S(0) &= 0 g/L \\ C_L(0) &= 6 mg/L \\ C_G(0) &= 250 mg/L\end{aligned}$$

Note: This system of ODEs is *stiff*, which roughly means that there are fast and slow processes in the system, making the numerical solution difficult. Because of this:

In MATLAB: use solver ode15s with the following options:

options = odeset('RelTol', 1e-6, 'AbsTol', 1e-6, 'nonnegative', [1:4]);

In Python: use the method 'BDF' within the solve_ivp from scipy:

solve_ivp(system_of_odes, t_span, y0, method='BDF', rtol=1e-6, atol=1e-6)

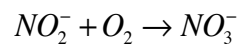
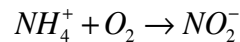
Do not forget to import the function: from scipy.integrate import solve_ivp

- Vary the feed volume flux between 6.5 and 10 L/h. Find a K_{La} value for each feed value so that your process is never oxygen limited and describe how you verified this. For feed flux of 10 L/h, plot the growth rate vs. the substrate concentration and comment on the growth kinetics.
- Operate the system as a batch reactor by setting $F = 0$ L/h and the initial substrate concentration 30 g/l. Consider $K_{La} = 70 h^{-1}$. Plot OUR and C_L over time and plot OUR versus S , describe and discuss your observation. What are the reasons for this behaviour.

- c) Measure the *OUR* from the difference between inlet and outlet gas phase oxygen concentrations. Compare the results with the ones you obtained in b) and explain the differences.
- d) Operate again as a CSTR with a feed volume flux of 6.5 L/h and simulate for substrate feed concentrations of 30 g/L and 100 g/L. Initial concentration for substrate in the tank is 0. Consider $K_{La} = 70 \text{ h}^{-1}$. Compare the oxygen uptake rate and C_L .

EXERCISE 3

Nitrification in a biofilm-fluidized bed reactor is to be modeled. The sequential oxidation of NH_4^+ to NO_2^- and NO_3^- proceeds according to:



Neglecting the details of the biofilm diffusion, the apparent kinetics of this biofilm process can be approximately described with homogeneous kinetics as it follows:

$$r_1 = v_{m1} \frac{S_1}{K_1 + S_1} \frac{C_L}{K_{O1} + C_L}$$

$$r_2 = v_{m2} \frac{S_2}{K_2 + S_2} \frac{C_L}{K_{O2} + C_L}$$

where S_1 stands for NH_4^+ , S_2 for NO_2^- , S_3 for NO_3^- and C_L for oxygen. The reaction starts with an initial amount of NH_4^+ equal to 100 mg/L and dissolved oxygen of 7 mg/L.

The parameter values of the process were estimated to be:

$$v_{m1} = 125 \text{ h}^{-1}; v_{m2} = 75 \text{ h}^{-1}; K_1 = 5.0 \text{ mg/L}; K_2 = 3.0 \text{ mg/L}; K_{O1} = 0.25 \text{ mg/L}; K_{O2} = 0.5 \text{ mg/L};$$

- a) Write the concentration balance in this batch system for S_1 , S_2 , S_3 and C_L .

$$Y_{O/S_1} = 3.5 \text{ mg/mg}; Y_{O/S_2} = 1.1 \text{ mg/mg}; k_{La} \in [1, 100] \text{ h}^{-1}, C_L^* = 8 \text{ mg/L}.$$

- b) Determine the k_{La} required to maintain C_L above the value of K_{O1} . For this, plot the dependency of C_L from k_{La} .
- c) What is the approximate time for NH_4^+ to go from 100 mg/L to zero if no oxygen limitation is present? Plot also the amounts of all 4 species of the system for the value of k_{La} that you found in b).