

## Course 28451: Optimizing Plantwide Operation

### *Exercise 4A: Dynamics & control of bioreactor: Linearisation*

This exercise deals with the linearisation of the dynamics of a bioreactor under a continuous operating regime. You will study important issues about the linearisation of dynamic systems such as the importance of linearising at steady-state (equilibrium point) and the validity range of linearised models. You will do so by simulating a simple model of a continuous fermentation bioreactor and using linearisation tools in Matlab.

#### The continuous fermentation model

The model described earlier in exercise 1 is to be used here as well. The system is depicted again in Figure 1.

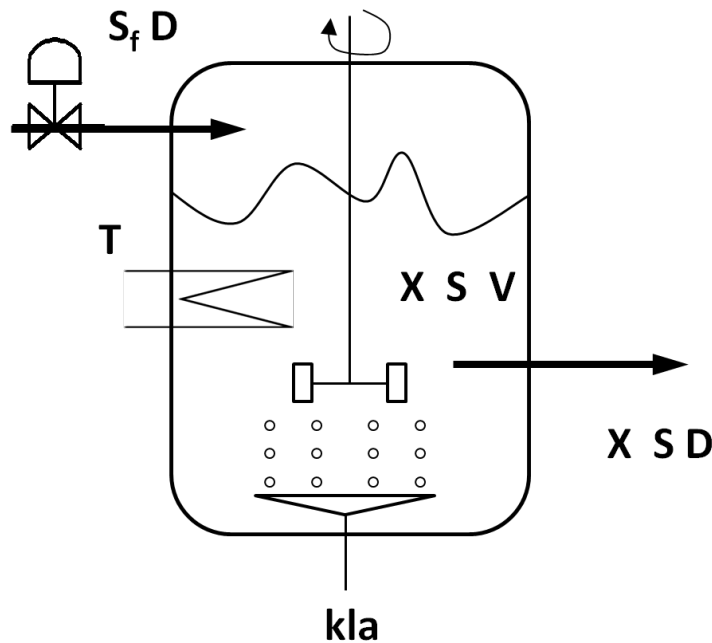


Figure 1: Continuous fermentation bioreactor

The specific growth rate,  $\mu$ , is given by double Monod kinetics:

$$\mu = \mu_{\max} \frac{S}{K_S + S} \frac{O}{K_O + O}$$

$K_S$  is the half saturation coefficient for carbon substrate (glucose),  $K_O$  the half saturation coefficient for oxygen and  $\mu_{\max}$  is the maximum specific growth rate. Material balances for the cell mass and the substrate, assuming an ideally mixed bioreactor and  $F_{in} = F_{out}$ , read as follows:

$$\begin{aligned}\frac{dX}{dt} &= \mu \cdot X - F/V \cdot X \\ \frac{dS}{dt} &= F/V \cdot (S_f - S) - \frac{1}{Y_{XS}} \mu \cdot X \\ \frac{dO}{dt} &= F/V \cdot (O_f - O) - \left( \frac{1}{Y_{XS}} - 1 \right) \mu \cdot X + k_l a \cdot (O^{sat} - O)\end{aligned}$$

Where  $Y_{XS}$  is the constant yield coefficient [g cells formed/g substrate consumed] which is assumed constant. In the following, the parameter values are  $V = 2$  L,  $F = 0.5$  L/h,  $K_S = 0.1$  g/L,  $K_O = 0.2 \times 10^{-3}$  g/L,  $Y_{XS} = 0.4$  g/g,  $k_{la} = 250$  h<sup>-1</sup> and  $S_f = 10$  g/L,  $O_f = 0$  g/L.

Temperature dependency of growth kinetics is given by the following Arrhenius relationship (refer to Villadsen et al., 2011):

$$\mu_{\max} = \frac{A \exp\left(-\frac{E_g}{RT}\right)}{1 + B \exp\left(-\frac{G_d}{RT}\right)} \quad \text{h}^{-1} \quad \text{for } 283.15 \text{ K} < T < 323.15 \text{ K}$$

Where  $A$  and  $B$  are Arrhenius constants respectively,  $E_g$  is the activation energy for growth and  $G_d$  is free energy change for deactivation of proteins/denaturation,  $R$  is the universal gas constant and  $T$  is temperature of the medium in Kelvin. The following parameter values for the microbial system are assumed:  $A = 1 \times 10^{10}$  (h<sup>-1</sup>);  $B = 3 \times 10^9$  (h<sup>-1</sup>);  $E_g = 58$  (kJ/mol);  $G_d = 550$  (kJ/mol);  $R = 8.314 \times 10^{-3}$  kJ/(mol\*K).

Mass transfer kinetics of oxygen from gas to liquid are also dependent on temperature through Henry coefficients. Hence the saturation concentration of oxygen in the medium is given by the following relationship (Villadsen et al., 2011):

$$\begin{aligned}O_{sat} &= P_{O_2} \cdot k_H \quad \text{mmol } O_2 / L \\ k_H &= 0.027 \exp\left(\frac{1142}{T}\right) \quad \text{mmol } O_2 / L \cdot \text{atm for } 298 \text{ K} < T < 324 \text{ K}\end{aligned}$$

Where  $O_{sat}$  is oxygen saturation concentration (in mmol/L),  $P_{O_2}$  is partial pressure of oxygen in air (0.21 atm at ambient temperature),  $k_H$  is henry coefficient for oxygen in water which depends on temperature, solute and medium characteristics. The nominal operation temperature of the bioreactor is set to 25 °C.

In this exercise, the following is asked:

1. Perform open loop simulations with the model of the system. Use the following initial conditions for the dynamic simulations [3 0 0]. You should use a long simulation time of this to be sure of your steady state with high numerical accuracy e.g. 100 hrs.
2. Linearise the system around the steady-state solution (equilibrium point). Simulate the system behaviour at this equilibrium point using the linear and nonlinear models e.g.

- a. Step responses in the inputs. Compare and explain the simulation results. What are the differences?
- b. Are the predictions of the linear model valid at initial conditions different than equilibrium? Simulate the linear model using different initial conditions (e.g.  $\pm 5\%$  around the equilibrium point).

This exercise forms part A of exercise 4. A written report on the combined results of exercise 4 part A and B with interpretation and discussion is to be handed in on DTU Learn as a single pdf file.

The report should contain a problem statement (you may rephrase the exercise), the results and interpretation / discussion of the results. The following is suggested for the documentation:

- A few representative plots (with appropriate titles and labels),
- A description of the solution procedure.
- Answers to the specific questions in the problem.