SIMULATION OF SIMPLE BIOREACTORS

Computer laboratory work in Wastewater Treatment – W4

1. Microbial growth in a ”Monode” reactor
2. Microbial growth in a ”Haldane” reactor
3. A simple activated sludge process

Preparation exercises:
1. Sec. 2, Exercise 2.1-2.3
2. Sec 3, Exercise 3.1
3. Sec. 4, Exercise 4.1

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1 Introduction

Modeling and simulation studies become more and more common in the biotechnical field including biological wastewater treatment. Typical applications of a simulation study are:

- Design of the process. The choice of size and configuration of a wastewater plant may be determined more easily by means of simulations. Also the impact of changing a plant configuration may be more easily predicted.

- Process control. Efficient control strategies are often model based. Also a good dynamic model can be used to test and evaluate different control strategies.

- Forecasting. Models can be used to predict future plant performance.

- Education. Models used in simulators can be used for education and training. This may require special types of simulators where the interface is adapted to the actual plant.

- Research. It is very common to use models and simulation studies to develop and test hypotheses in all kinds of research work.

In all simulation studies it is of fundamental importance to be aware of model approximations and the validity of the model. Note that different needs often lead to different requirement of the accuracy of the underlying model.

In this laboratory work you will first simulate two types of simple bioreactor using a Java applet designed for this purpose. You will study how different flows, growth rates, and concentrations affect the process. Finally, an activated sludge process for carbon removal is studied (in the next computer lab. work you will study a more complex model, based on the Activated Sludge Model No 1).

2 Microbial growth in a Monode reactor

2.1 The model

We will consider the dynamics of a completely mixed tank reactor shown in Figure 1. The influent flow rate is equal to the effluent flow rate $Q$ [volume/time]. Hence, the volume $V$ is constant. The dilution rate is $D = \frac{Q}{V}$. The influent has a substrate concentration $S_{in}$ [mass/volume]. The influent biomass is assumed to be neglectable ($X_{in} = 0$).
The biomass growth in the reactor is assumed to follow the Monod kinetics

\[
\mu(S) = \mu_{\text{max}} \frac{S}{K_S + S}
\]

(1)

where

- \( \mu_{\text{max}} \) is the maximum specific growth rate
- \( S \) is the concentration of substrate
- \( K_S \) is the half saturation constant

For the substrate consumption we assume that the yield is \( Y \).

By applying a mass balance, the following dynamic model can be derived \(^1\)

\[
\frac{dX}{dt} = (\mu(S) - D)X
\]

\[
\frac{dS}{dt} = -\frac{1}{Y} \mu(S)X + D(S_{\text{in}} - S)
\]

(2)

### 2.2 Exercises

**Exercise 2.1** Derive the stationary values\(^2\) \((\bar{X}, \bar{S})\) of the biomass and substrate concentration from (1)–(2). Also show how the yield factor \( Y \) can be estimated from knowledge of \( \bar{X}, \bar{S} \) and \( S_{\text{in}} \).

**ANSWER:**

\(^1\)A derivation can be found in the course material "An introduction to modeling of bioreactors".

\(^2\)This is obtained by solving \(\frac{dX}{dt} = \frac{dS}{dt} = 0\).
Exercise 2.2 The definition for wash-out (all biomass is washed out from the reactor) is $\dot{X} = 0$. What is the corresponding value on $\dot{S}$?

**ANSWER:**

Exercise 2.3a Calculate a limit $D_{lim}$ so that if $D \geq D_{lim}$ wash out will occur. Hint: The condition for non wash-out is that $S_{in} > \dot{S}$, where $\dot{S}$ is calculated in Exercise 2.1.

**ANSWER:**

Exercise 2.3b Calculate numerically the stationary values $\dot{X}$ and $\dot{S}$ (see Exerc. 2.1) and $D_{lim}$ (see Exerc. 2.3a) for the case: $\mu_{max} = 2$, $K_S = 1.2$, $Y = 0.8$, $S_{in} = 1$ and $D = Q/V = 0.5$. (the units are “appropriate”)

**ANSWER:**

Exercise 2.4 Next you shall use a small simulation program written as a Java applet. The simulator has the default values given in Exec 2.3b. The initial\(^3\) values are: $X_0 = 0.1$, $S_0 = 1.1$.

The default simulation length $T_{max}$ is 40 time units.

To run the simulator, start Netscape and go to the following URL: http://www.syscon.uu.se/JASS

Select the link Bioreactors in the table.

The applet has three tabs. Select the Mode tab. From the plot, estimate the stationary values of biomass and substrate. Also estimate the yield factor from those values. Compare the results with the calculated values in Exercise 2.3b.

\(^3\)The concentrations at time $t=0$ in the reactor, these values should not affect the final concentrations if the simulation length is sufficiently long.
Exercise 2.5 Increase the value of $D$ until wash-out is obtained. For what value on $D$ is wash-out obtained? Compare with Exercises 2.3b. Compare also $S$ with the result in Exercise 2.2.

Exercise 2.6, Optional Check how the simulated biomass and substrate is affected by different values on $\mu_{max}$, $K_S$, $Y$, $S_{in}$ and $D = Q/V$

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4The exact value may be hard to see from the plot, increase the simulation time if necessary.
3 Microbial growth in a Haldane reactor

3.1 The model

In this section we will briefly consider the case when the same tank configuration as in the previous section is used but the biomass growth is modeled with the Haldane kinetics

$$\mu(S) = \mu_0 \frac{S}{K_1 + S + S^2/K_h}$$  (3)

Here, $\mu_0$, $K_1$ and $K_h$ are parameters describing the growth rate. This model takes into account possible substrate inhibitory effects at high concentrations of the substrate.

3.2 Exercises

Exercise 3.1 The Haldane law gives two possible stationary values of the substrate denoted $\tilde{S}_1$ and $\tilde{S}_2$. See Exercise 1 in "Räkneuppgifter V". Calculate $\tilde{S}_1$ and $\tilde{S}_2$ for the case:

$\mu_0 = 1.5$, $K_1 = 1.2$, $K_h = 2$, $Y = 0.8$, and $D = Q/V = 0.5$.

**ANSWER:**

The simulator has the following default values

$\mu_0 = 1.5$, $K_1 = 1.2$, $K_h = 2$, $Y = 0.8$, and $D = Q/V = 0.5$, $S_{in} = 1$.

From the user interface, the above parameters can be changed except $\mu_0$ which is fixed to 1.5. The initial values are: $X_0 = 0.5$, $S_0 = 0.5$.

Exercise 3.2 In the simulator, select the tab labeled *Haldane*. From the plot, estimate the stationary values of the substrate and verify that one of the possible stationary points calculated in Exercise 3.1 is achieved.

**ANSWER:**
**Exercise 3.3** Check the stationary value of $S$ for different input concentrations $S_{in}$ and notify conditions for wash-out. Does wash out only occur for low values of $S_{in}$? Explain!

**ANSWER:**

Concluding remarks: A basic feature of many nonlinear systems like bioreactor models is that the stationary points can be stable or unstable. For the Haldane example above, only one stationary point is stable. In order to further analyze this behavior, phase plane representation may be useful, compare with the course in ODE.

## 4 A simple activated sludge process

In this exercise you will study a simple model for an activated sludge process.

### 4.1 The model

The process to be modeled is a simple activated sludge process with recycled sludge and wasting (removal of excess sludge) from the recycle line. In the clarifier, the biomass is separated from the treated water. A layout of the process is shown in Figure 2.

![Figure 2: Representation of a completely mixed activated sludge process](image)

The biomass growth in the aeration tank is modeled as

$$V \frac{dX}{dt} = \mu VX + Q_r X_r - (Q_{in} + Q_r)X$$

where

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

The substrate consumption is modeled as

$$V \frac{dS}{dt} = -\frac{1}{Y} \mu VX + Q_m S_{in} + Q_r S_r - (Q_{in} + Q_r)S$$
The sedimentation model is

\[
(Q_{\text{in}} + Q_r)X = (Q_r + Q_w)X_0 \quad \text{and} \quad S = S_e = S_r \quad \text{and} \quad Q_e = Q_{\text{in}} - Q_w
\]

The expression for the sludge age in an ideal settler is (see "See Exercise 5 in Räkneuppgifter V"):

\[
\theta_s = V \frac{Q_r + Q_w}{Q_w(Q_{\text{in}} + Q_r)}
\]  

(4)

Note that \( \theta_s \) does not depend on the sludge content \( X \).

4.2 Exercises

**Exercise 4.1a** Derive the stationary values (\( \bar{X}, \bar{S} \)). \( \bar{S} \) should be written as a function of sludge age \( \theta_s \), \( \mu_{\text{max}} \) and \( K_S \). \( \bar{X} \) should be written as a function of the sludge age \( \theta_s \), yield \( Y \), \( D = Q_{\text{in}} / V \) and \( S_{\text{in}} - \bar{S} \).

Hints:
Use the sedimentation model to simplify the biomass and substrate models.
Use the steady state relation between sludge age and specific growth rate (this will directly give \( \bar{S} \)).

**ANSWER:**

In the simulator the following values are fixed:
\( \mu_{\text{max}} = 6/24 \text{ h}^{-1} \), \( K_S = 20 \), and \( Y = 0.8 \).

The following parameters can be changed from the program interface, their nominal values are also given:

- Inflow \( Q_{\text{in}} = 2000 \text{ m}^3/\text{h} \)
- Return sludge flow: \( Q_r = 2000 \text{ m}^3/\text{h} \)
- Excess sludge flow rate \( Q_w = 83 \text{ m}^3/\text{h} \)
- Aerated basin volume \( V = 4000 \text{ m}^3 \)
- BOD concentration in influent water : \( S_{\text{in}} = 150 \text{ g/m}^3 \)

In the simulator the sludge age is presented using the unit days (common practice). Remember to make the necessary unit conversions.
Exercise 4.1b Calculate numerically the stationary values $\bar{X}$ and $\bar{S}$, and the sludge age $\theta_s$ using the nominal values above.

**ANSWER:**

Exercise 4.2 In the simulator, select the tab labeled ASP. From the plot, estimate the stationary values of biomass and substrate. Compare the simulated results with the ones obtained from Exercise 4.1.b.

**ANSWER:**

Straightforward manipulations of (4) gives

$$Q_w = \frac{V}{2\theta_s - \frac{V}{Q_{in}}}$$  \hspace{1cm} (5)

which shows how $Q_w$ should be selected to give a desired sludge age.

During a non-trivial steady state, we must have that\(^5\)

$$\theta_s = \frac{1}{\mu(S)}$$  \hspace{1cm} (6)

\(^5\)See, the course material "An introduction to modeling of bioreactors".
Exercise 4.3 Select a desired value (less than $S_{in}$) of the effluent substrate $\tilde{S}$. Then use (6) to calculate the needed sludge age and (5) to find the excess sludge flow rate $Q_w$. Simulate the process with this choice of $Q_w$ and check if the system behaves as expected. Try some different substrate levels. What happens with the biomass concentration when $\tilde{S}$ is decreased?

\textbf{Answer:}

Exercise 4.4 Calculate the limiting sludge age which gives wash out. Simulate the process using this sludge age and verify that wash out is achieved. Try also slightly larger and smaller values. Comment shortly on the result.

Hint: The limiting condition for wash-out is $\tilde{S} = S_{in}$.

\textbf{Answer:}

Exercise 4.5 - Optional Play around with the simulator, try different parameter values, for example, effects of volume changes. Try to predict the simulation results by using the previously derived equations.

\textbf{Answer:}

\[\text{Due to the discrete character of the slide bar in the user interface it may be impossible to exactly implement the desired flow rate.}\]