An introduction to modeling of bioreactors

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Abstract

This material is made for the course "Wastewater treatment" in the Aquatic and Environmental Engineering program. The sections which are marked with a $*$ are not central in the course.

Contents

1 Background

Mathematical models are an important tool also in wastewater treatment. Typical general applications include

- Design of the process. A model is then helpful in evaluating the impact of changing system parameters etc. It is, however, fair to mention that often empirical rules or thumb rules are used in design of wastewater treatment plants.
- Process control. Efficient control strategies are often model based.
- Forecasting. Models can be used to predict future plant performance.
- Education. Models used in simulators can be used for education and training.
- Research. Development and testing of hypotheses.

Below we will derive some simple models for bioreactors (including the activated sludge process). Such models can help explain some fundamentals properties of bioreactors and also give suitable background for understanding more advanced models like the IAWQ

model no 1.

Even if we in this course mainly focus on the use of bioreactors for treatment of wastewater it is fair to mention that the bioreactors are used in many other applications including industries concerned with food, beverages and pharmaceuticals. Biotechnology, which deals with the use of living organisms to manufacture valuable products, has had a long period of traditional fermentations (production of beer, wine, cheese etc.). The development of microbiology, around hundred years ago, expanded the use of bioreactors to produce primary metabolic products. In 1940's the large scale production of penicillin was a major breakthrough in biotechnology. Some 20 years ago, the computer technology started to make advanced process control possible. The development of genetic engineering have played a major role in creating the current progress in the field of biotechnology.

Until recently, the biotechnical industry has been lagged behind other industries in implementing control and optimization strategies. A main bottleneck in biotechnological process control is the problem to measure key physical and biochemical parameters.

2 The specific growth rate

Many biochemical processes involves (batch) growth of microorganisms. After adding living cells to a reactor containing substrate[1], one may distinguish four phases, see also Figure 1:

- A lag phase when no increase in cell numbers is observed.
- An exponential growth phase.
- A stationary phase.
- A death phase. The number of cells decreases due to food shortage.

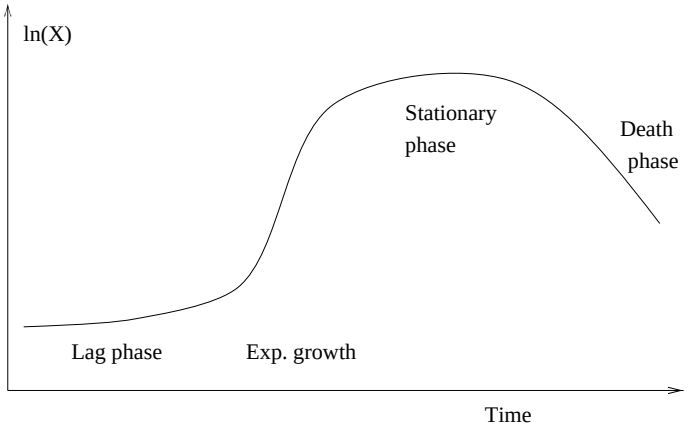

Figure 1: Typical bacterial growth curve.

Next we will consider the exponential growth phase. Let $X(t)$ denote the concentration of biomass population (mass/unit volume). An exponential growth can be expressed as

$$\frac{dX(t)}{dt} = \mu X \tag{1}$$

[1]Substrate is defined as the source of energy, it can be organic (for heterotrophic bacteria), inorganic (e.g. ammonia), or even light (for phototrophs).

The parameter μ is denoted the *specific growth rate*, "rate of increase in cell concentrations per unit cell concentrations" ([1/time unit]).

2.1 Derivation

For completeness we give a derivation of (1) commonly used in microbiology literature.

An exponential growth means that the concentration (or number of cells) is doubled during each fixed time interval. Hence, $X(t)$ can be expressed as

$$X(t) = X_o 2^{(t-t_o)/t_d} \tag{2}$$

where t_d is the doubling time and X_o is the initial concentration at time $t = t_o$. Logarithming both sides gives

$$\frac{\ln X(t) - \ln X_o}{t - t_o} = \frac{1}{t_d} \ln 2 \tag{3}$$

Let, $t \to t_o$, the use of the definition of the derivative then gives

$$\frac{d}{dt} \ln X(t) = \frac{1}{t_d} \ln 2 \tag{4}$$

Now, since

$$\frac{d}{dt} \ln X(t) = \frac{1}{X(t)} \frac{dX(t)}{dt} \tag{5}$$

we have

$$\frac{1}{X(t)} \frac{dX(t)}{dt} = \frac{1}{t_d} \ln 2 = \mu \tag{6}$$

which can be written in the standard form (1).

3 The Monod function

Often the growth rate is limited by substrate. The following empirical relation is often used and is commonly named the *Monod function*[2]

$$\mu = \mu_{max} \frac{S}{K_S + S} \tag{7}$$

where

μ_{max} is the maximum specific growth rate
S is the concentration of growth limiting substrate
K_S is the half saturation constant

The effect of the substrate concentration on the specific growth rate is shown in Figure 2.

[2]It was initially proposed by Michaelis-Menton in 1913 (the relation is therefore also often called Michaelis-Menton law) and extended by Monod in 1942 to describe growth of microorganisms.

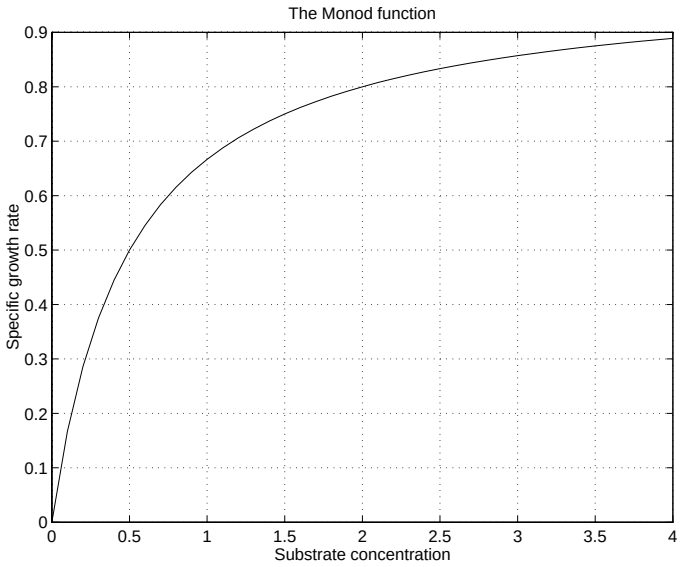

Figure 2: Illustration of the Monod function. The following parameters are used $K_S = 0.5$ and $\mu_{max} = 1$. Note that $S = K_S$ gives $\mu = 0.5\mu_{max}$.

As the microorganisms increase, substrate is used. This is commonly expressed as:

$$\frac{dX}{dt} = -Y\frac{dS}{dt} \tag{8}$$

where Y is the *yield coefficient*, "the ratio of the mass of cells formed to the mass of substrate consumed". The yield coefficient can be expressed as

$$Y = -\frac{dX}{dS} \tag{9}$$

In the literature, it is common to "neglect" the minus sign in the definition of Y and/or to consider the inverse of the yield coefficient.

4 Microbial growth in a stirred tank reactor

We will consider the dynamics of a completely mixed tank reactor shown in Figure 3. The influent flow rate is equal to the effluent (output) flow rate Q [volume/time]. Hence, the volume V is constant. The influent has a substrate concentration S_{in} [mass/volume]. No influent biomass is assumed.

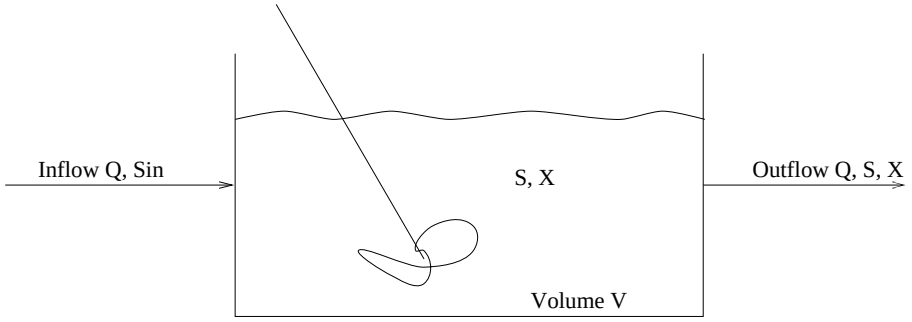

Figure 3: A completely mixed bioreactor.

The rate of accumulation of biomass is obtained from a mass balance. Assume that the biomass has a specific growth rate of μ. The total amount of produced biomass per time unit in a reactor with volume V is μVX, cf (1). Since the reactor is completely mixed, the outflow concentration of biomass is equal to the concentration in the tank. The rate of change of biomass is then given as

$$V\frac{dX}{dt} = \mu VX - QX \tag{10}$$

Now, define the *dilution rate*

$$D = \frac{Q}{V} \tag{11}$$

The model (10) can now be written in the following simple form

$$\frac{dX}{dt} = (\mu - D)X \tag{12}$$

For the substrate consumption we assume that the yield is Y, see (8). Paralleling, the procedure above for the substrate mass balance gives

$$V\frac{dS}{dt} = QS_{in} - \frac{\mu}{Y}VX - QS \tag{13}$$

Introducing the dilution rate (11) gives

$$\frac{dS}{dt} = -\frac{\mu}{Y}X + D(S_{in} - S) \tag{14}$$

The model consisting of (12) and (14) form the basis for most bioreactors models including the activated sludge process.

Typical extensions of the model are

- The use of a specific grow rate which depends on several variables S_1, S_2, ... S_n (substrates and nutrients). That is

$$\mu = \mu_{max}\prod_{n=1}^{N}\frac{S_n}{K_{S,n} + S_n} \tag{15}$$

See, for example, the IAWQ model no 1. Note also that other environmental factors like pH and temperature affect the growth rate. This may be modeled in a similar way. It is also common that a substance, say S_i, has an inhibitory effect at high concentrations. This may be modelled as

$$\mu_i = \frac{K_i}{K_i + S_i} \tag{16}$$

If $S_i >> K_i$ then μ_i is close to zero. A typical example is the modelling of anoxic growth of heterotrophs. Then S_i corresponds to the concentration of dissolved oxygen in the water.

- The Monod function (7) does not account for any inhibitory effects at high substrate concentrations (overloading). Substrate inhibition may be modeled by the *Haldane* law

$$\mu = \frac{\mu_o S}{K_M + S + K_I S^2} \tag{17}$$

It is clearly seen in (16) that $\mu \to 0$ as $S \to \infty$.

- The use of different substrate and biomass compounds. Very often the oxygen consumption is included in the model.

- Conversion relations between different compounds, i.e. hydrolysis[3].

- A decay term for biomass can be added to account for the death of microorganisms. The specific biomass decay rate b is defined similarly as the specific growth rate μ:

$$b = -\frac{dX(t)}{Xdt} \tag{18}$$

The net growth rate is then $\mu - b$ and (12) becomes

$$\frac{dX}{dt} = (\mu - b - D)X \tag{19}$$

Finally, it is worth mentioning that COD (chemical oxygen demand) is often used (g COD/m^3) since it gives a consistent description when oxygen is used as a model parameter.

4.1 State space description and stationary points

The model consisting of (12) and (14) can easily be written in a state space form. Define the state space vector as

$$z(t) = \begin{pmatrix} X(t) \\ S(t) \end{pmatrix}$$

Let X be the output (denoted $y(t)$) and S_{in} be the input signal. The model (12)–(14) can now be written as

$$\begin{aligned} \dot{z}(t) &= \begin{pmatrix} \mu - D & 0 \\ -\frac{\mu}{Y} & -D \end{pmatrix} z(t) + \begin{pmatrix} 0 \\ D \end{pmatrix} S_{in} \\ y(t) &= \begin{pmatrix} 1 & 0 \end{pmatrix} x(t) \end{aligned} \tag{20}$$

[3]In the hydrolysis process, larger molecules are converted into small degradable molecules.

The model (20) is linear if μ, Y, and D are constant. This is rarely the case! The model can be linearized around a *stationary point* (also called equilibrium state or fixed point) X_o, S_o obtained from solving $\dot{z} = 0$.

Assume D is constant. If we look at $X(t)$ (the first component of z), it is seen that a necessary condition for $\dot{z} = 0$ is

$$X_o = 0 \tag{21}$$

or

$$\mu = D \tag{22}$$

The first condition (21) is known as *wash-out*. All biomass will disappear! In most cases the wash-out condition is undesirable and should be avoided. If $D > \mu$, the only possible stationary point is (21). This means that, initially, more biomass is taken out from the system than is produced. Note that, the corresponding S_o for the condition (21) is $S_o = S_{in}$ which is very natural. Why?

4.2 Different flow rates*

In the case the influent flow rate is different from the effluent flow rate, the volume variation in the reactor need to be taken into account:

$$\frac{dV}{dt} = Q_{in} - Q_{out} \tag{23}$$

where Q_{in} is the influent flow rate and Q_{out} the effluent flow rate.
A mass balance for the biomass yields

$$\frac{d}{dt}(VX) = \mu VX - Q_{out}X \tag{24}$$

By applying the chain rule, we have

$$\frac{d}{dt}(VX) = X(\frac{d}{dt}(V) + V(\frac{d}{dt}X) = X(Q_{in} - Q_{out}) + V(\frac{d}{dt}X)$$

In the last equality, (23) has been used. Rearranging the terms gives

$$V\frac{dX}{dt} = \frac{d}{dt}(VX) + (Q_{out} - Q_{in})X \tag{25}$$

Inserting (24) in (25) gives

$$V\frac{dX}{dt} = \mu VX - Q_{in}X \tag{26}$$

For this case, it is feasible to define the dilution rate as

$$D = \frac{Q_{in}}{V} \tag{27}$$

The model (26) can now be written in the following simple form

$$\frac{dX}{dt} = (\mu - D)X \tag{28}$$

which is the same as (12), given the (more careful) definition of the dilution rate in (27).

For the substrate concentration, a similar modeling exercise can be done. The results is the same as (14).

5 The activated sludge process

In this section we will apply the basic models derived in Section 4, to 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 4. In the aeration tank, air flow is feed in order to supply the microorganisms with oxygen. Here, we will not model this oxygen consumption. Instead it is assumed that enough oxygen is available.

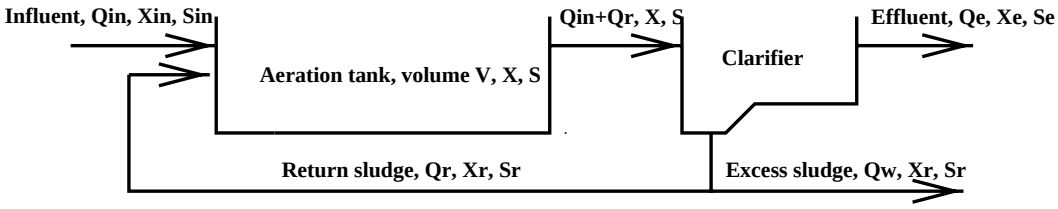

Figure 4: Schematic representation of a completely mixed activated sludge process. Flow rates are denoted Q, substrate concentration S, and biomass (microorganism concentration) X.

In the basic layout in Figure 4 we assume that

$$Q_{in} = Q_e + Q_w$$

That is, the water volume is constant.

Applying a mass balance for the aeration tank depicted in Figure 4, gives

$$V\frac{dX}{dt} = Q_{in}X_{in} + Q_rX_r + \mu VX - (Q_{in} + Q_r)X \tag{29}$$

For the clarifier we assume that

- No biological reactions take place.
- The dynamics can be neglected.

The following mass balance then holds for the clarifier

$$(Q_{in} + Q_r)X = (Q_r + Q_w)X_r + Q_eX_e \tag{30}$$

It is often reasonable to set $S = S_r = S_w = S_e$ ie the concentration of the substrate is assumed soluble and unaffected by the sedimentation. This is generally assumed for all soluble components.

Using (30) in (29) gives

$$V\frac{dX}{dt} = Q_{in}X_{in} + \mu VX - (Q_eX_e + Q_wX_r) \tag{31}$$

Normally, X_{in} is much smaller than the biomass concentration in the system and can therefore be neglected. Hence, we assume $X_{in} = 0$. We can thus write (31) as

$$V\frac{dX}{dt} = \mu VX - (Q_eX_e + Q_wX_r) \tag{32}$$

A model for the substrate consumption can be derived in a similar way.
Next, consider the steady state condition ($\frac{dX}{dt} = 0$) and assume a stationary value of $X > 0$. We then obtained from (32)

$$\frac{1}{\mu} = \frac{VX}{Q_e X_e + Q_w X_r} \tag{33}$$

The right hand side of (33) is known as the *sludge age* and is denoted θ_s ie

$$\theta_s = \frac{VX}{Q_e X_e + Q_w X_r} \tag{34}$$

Other names for θ_s is biological solids retention time and mean cell residence time.
The sludge age is the average time that the biomass is in the system. It can be expressed as

$$\theta_s = \frac{\text{Total mass of biomass in the aeration tank}}{\text{removed biomass per time unit}}$$

and it is often expressed in the time unit days.

If $\mu < \frac{1}{\theta_s}$, the consequence is *wash out*. Then more biomass is taken out from the system than is produced, cf the discussion in Section 4.1. Hence, the sludge age is one of the key parameters in the operation of an activated sludge process. For example, nitrifying bacteria has a relatively low growth rate. It is then necessary to have a high sludge age to obtain nitrification in the system. During winter time one may need a sludge age around 15-20 days for obtaining nitrification.