

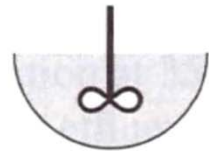
Reactors I

Today's lecture

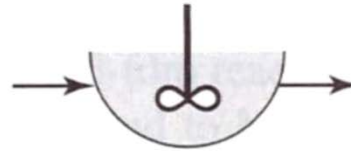
- Types of reactors
- Generic approach for reactor analysis
- Reactor analysis example: batch reactor
 - Batch reactor analysis for 1st order reaction
 - Batch reactor analysis for Monod kinetics
(with some knowledge buildup for numerical analysis)

Reactors

Suspended growth:



Batch reactor

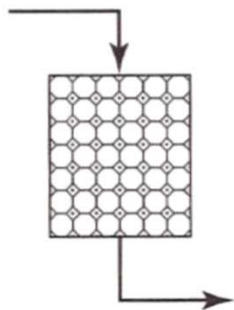


Continuous-stirred
tank reactor

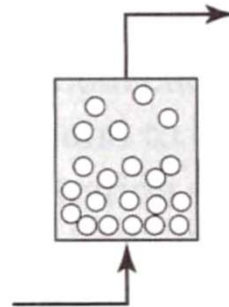


Plug-flow reactor

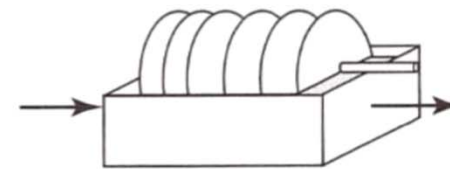
Attached growth:



Packed-bed reactor



Fluidized-bed reactor



Rotating biological contactor

Suspended vs. attached growth



suspended growth



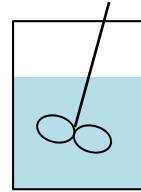
attached growth

Reactors for suspended growth

- **Batch reactor**

- Bench-scale test systems

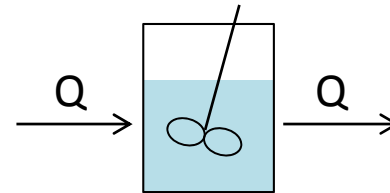
- Some wastewater processes – “sequencing batch reactors”



- **Continuous-stirred tank reactor (CSTR)**

- Activated sludge

- Flocculator



- **Plug flow reactor (PFR)**

- Disinfection

- Long river/canal

- Pipeline/aqueduct



Reactor analysis

1. Draw schematics and define control volume

2. Set mass balance (for a single substance!!!)

(mass rate of accumulation)

= (rate of mass in) – (rate of mass out)

+ (mass rate of gain/loss)



Any processes related to gain/loss, but here we are interested in reactions!

3. Rearrange/solve the equation to a useful form

Reactor analysis: batch reactor

For 1st order reaction of a contaminant,
(initial concentration = C_0)

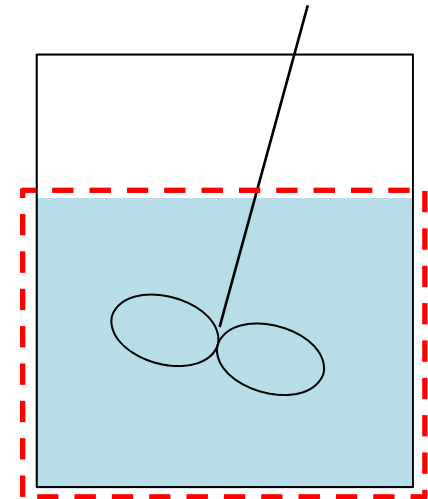
1) Draw schematics & define CV:
the entire reactor as CV

2) Set mass balance (for the contaminant)

$$\frac{dC}{dt} = -kC$$

3) Rearrange/solve

$$C/C_0 = e^{-kt}$$



Reactor analysis: batch reactor

For bacterial growth following Monod kinetics

2) Set mass balance (one for substrate, one for active biomass)

$$\frac{dS}{dt} = r_{ut} = -\frac{\hat{q}S}{K + S}X_a \quad (\text{substrate mass balance})$$

$$\frac{dX_a}{dt} = \mu X_a = \left(Y \frac{\hat{q}S}{K + S} - b \right) X_a = r_{net} \quad (\text{active biomass mass balance})$$

r_{net} = net rate of active biomass growth ($M_x L^{-3} T^{-1}$)

Batch reactor, Monod kinetics

3) Rearrange/solve

We need to get a solution for...

Governing equations

$$\frac{dS}{dt} = -\frac{\hat{q}S}{K+S}X_a$$

$$\frac{dX_a}{dt} = \left(Y \frac{\hat{q}S}{K+S} - b \right) X_a$$

Initial conditions

$$S(t=0) = S^0 \quad X_a(t=0) = X_a^0$$

Batch reactor, Monod kinetics

We would prefer $S = f(t)$, $X_a = g(t)$

The math here is much more difficult than it was for 1st order reaction because:

- There are two variables which are inter-correlated
- The differential equations are nonlinear with respect to S

Two ways of solving a mathematical model:

- 1) Analytical solution** – an exact solution
 - such as $S = f(t)$, $X_a = g(t)$; not always available
- 2) Numerical solution** – an approximate solution

Batch, Monod – Numerical solution

$$\frac{dS}{dt} = -\frac{\hat{q}S}{K+S}X_a \quad \frac{dX_a}{dt} = \left(Y \frac{\hat{q}S}{K+S} - b \right) X_a$$

Divide the time range into finite time steps with a length of Δt .

Then, between n^{th} and $n+1^{\text{th}}$ time step, the 1^{st} derivatives can be approximated as:

$$\frac{dS}{dt} \approx \frac{S^{n+1} - S^n}{\Delta t} \quad \frac{dX_a}{dt} \approx \frac{X_a^{n+1} - X_a^n}{\Delta t} \quad S^n \text{ \& } X_a^n: S \text{ \& } X_a \text{ values at } n^{\text{th}} \text{ time step, respectively}$$

If n^{th} time step data are used for the right hand sides of the equations it is called as an “explicit” method.

cf) “implicit” method uses $n+1^{\text{th}}$ time step

Batch, Monod – Numerical solution

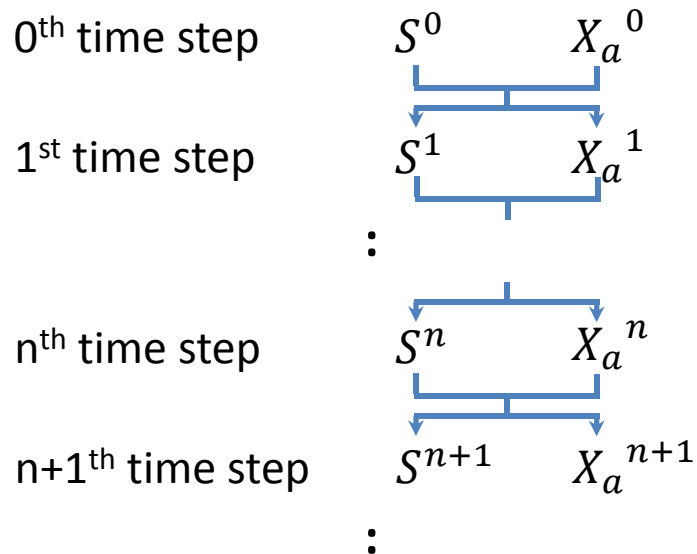
Let's try explicit method:

$$\frac{S^{n+1} - S^n}{\Delta t} = -\frac{\hat{q}S^n}{K + S^n} X_a^n \quad \Rightarrow$$

$$S^{n+1} = \left(1 - \frac{\hat{q}}{K + S^n} X_a^n \Delta t\right) S^n$$

$$\frac{X_a^{n+1} - X_a^n}{\Delta t} = \left(Y \frac{\hat{q}S^n}{K + S^n} - b\right) X_a^n \quad \Rightarrow$$

$$X_a^{n+1} = \left\{1 + \left(Y \frac{\hat{q}S^n}{K + S^n} - b\right) \Delta t\right\} X_a^n$$



Homework#3

Construct an Excel spreadsheet to predict the substrate and biomass concentration for a batch-type bioreactor by the numerical method.

What are the substrate and biomass concentrations after 0.1 d calculated by setting the following values as Δt ?

i. $\Delta t = 0.0001$ d; ii. $\Delta t = 0.001$ d; iii. $\Delta t = 0.05$ d

Use the following parameters:

$$S^0 = 500 \text{ mg COD/L}, \quad X_a^0 = 100 \text{ mg VSS/L}, \quad \hat{q} = 20 \text{ g VSS/g COD} - d$$
$$K = 100 \text{ mg COD/L}, \quad Y = 0.4 \text{ g VSS/g COD}, \quad b = 0.1/d$$

Homework#3

Compare the results for the numerical solution with different Δt values. In your opinion, which will be more accurate? Why? For $\Delta t = 0.05$ d, obtain the solutions for substrate and biomass concentrations at 0.5 d. What do you get?