Reactors I

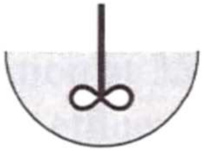
Today’s lecture

- 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

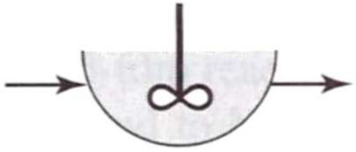
    (with some knowledge buildup for numerical analysis)

Reactors

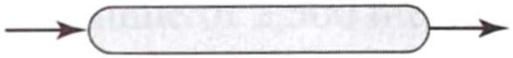
Suspended growth:



Batch reactor

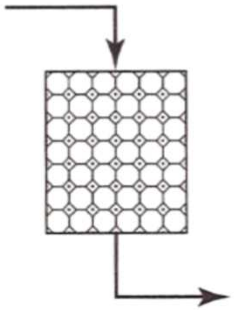


Continuous-stirred tank reactor

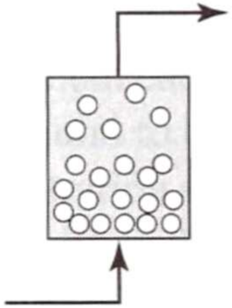


Plug-flow reactor

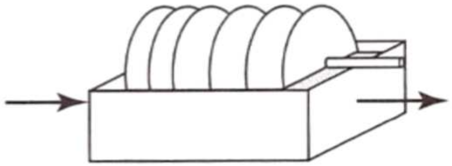
Attached growth:



Packed-bed reactor



Fluidized-bed reactor



Rotating biological contactor

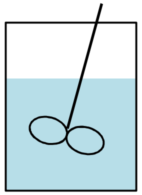
Suspended vs. attached growth

suspended growth

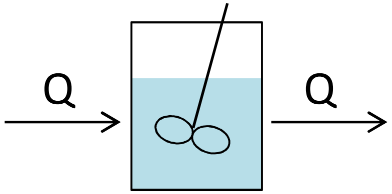
attached growth

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)

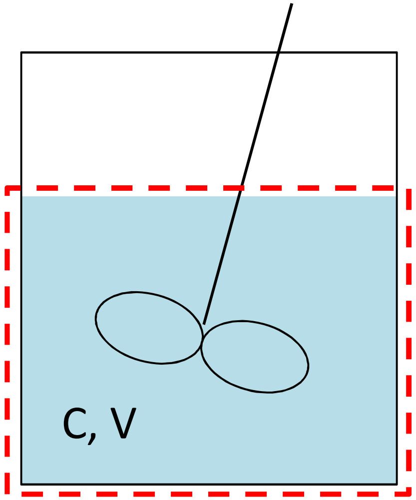
+ (mass rate of gain/loss)

↑

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

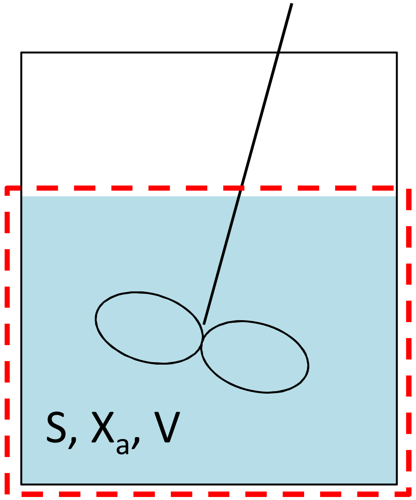
$$\boxed{C/C_0 = e^{-kt}}$$

Reactor analysis: batch reactor

For bacterial growth following Monod kinetics

2) Set mass balance

(one for substrate, one for active biomass)



[substrate mass balance]

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

[active biomass mass balance]

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

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

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

$$S(t=0) = S^0 \qquad X_a(t=0) = {X_a}^0$$

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 – Analytical solution

We need an assumption which is only occasionally acceptable that decay is negligible.

Then,

$$X_a = {X_a}^0 + Y(S^0 - S) \qquad \text{(biomass growth) = (true yield) x (substrate utilized)}$$

The two mass balance equations are reduced to one nonlinear differential eq.:

$$\frac{dS}{dt} = -\frac{\hat{q}S}{K+S}\left[{X_a}^0 + Y(S^0 - S)\right]$$

Using the best knowledge of math, we get:

$$t = \frac{1}{\hat{q}}\left\{\left(\frac{K}{{X_a}^0 + YS^0} + \frac{1}{Y}\right) ln\left({X_a}^0 + YS^0 - YS\right) - \left(\frac{K}{{X_a}^0 + YS^0}\right) ln\frac{S{X_a}^0}{S^0} - \frac{1}{Y} ln{X_a}^0\right\}$$

[5.11]

We fail to get an explicit solution of ***S*** as a function of ***t***

Batch, Monod – Numerical solution

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

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

Then, between nth and n+1th time step, the 1st derivatives can be approximated as:

$$\frac{dS}{dt} \approx \frac{S^{n+1} - S^{n}}{\Delta t} \qquad \frac{dX_a}{dt} \approx \frac{{X_a}^{n+1} - {X_a}^{n}}{\Delta t}$$

S^n & ${X_a}^n$: S & X_a values at nth time step, respectively

If nth time step data are used for the right hand sides of the equations it is called as an “explicit” method.

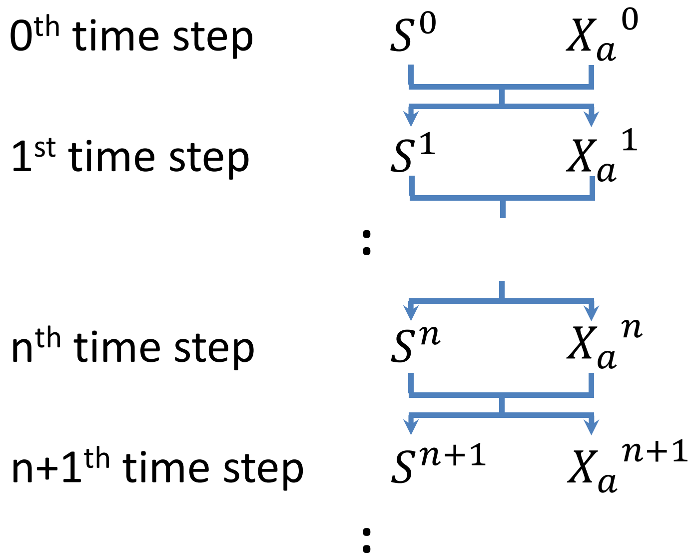
cf) “implicit” method uses n+1th time step

Batch, Monod – Numerical solution

Let’s try explicit method:

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

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



0th time step S^0 ${X_a}^0$

1st time step S^1 ${X_a}^1$

:

nth time step S^n ${X_a}^n$

n+1th time step S^{n+1} ${X_a}^{n+1}$

:

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. Δt = 0.0001 d; ii. Δt = 0.001 d; iii. Δt = 0.05 d

Use the following parameters:

$S^0 = 500\ mg\ COD/L,\ \ X_a{}^0 = 100\ mg\ VSS/L,\ \ \hat{q} = 20\ g\ VSS/g\ COD - d$

$K = 100\ mg\ COD/L,\ \ Y = 0.4\ \ g\ VSS/g\ COD,\ \ b = 0.1/d$

Homework#3

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