Reactors I

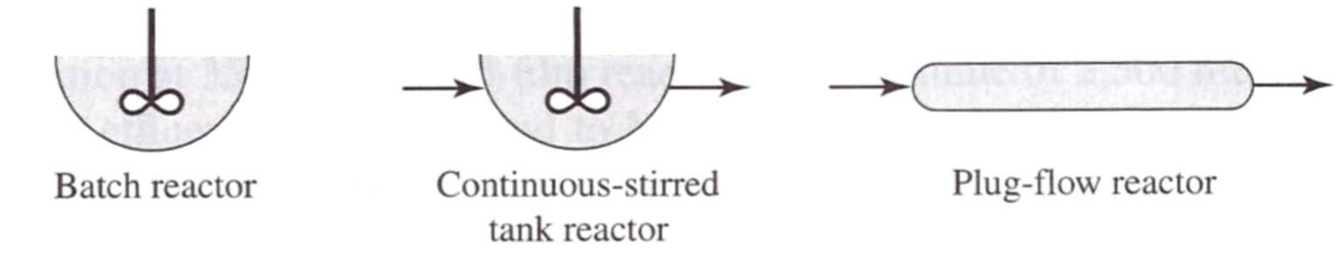
Today's lecture

- Types of bioreactors
- Generic approach for reactor analysis
- Reactor analysis example: batch reactor
  - Batch reactor analysis for 1st order reaction
  - Batch reactor analysis for Monod kinetics

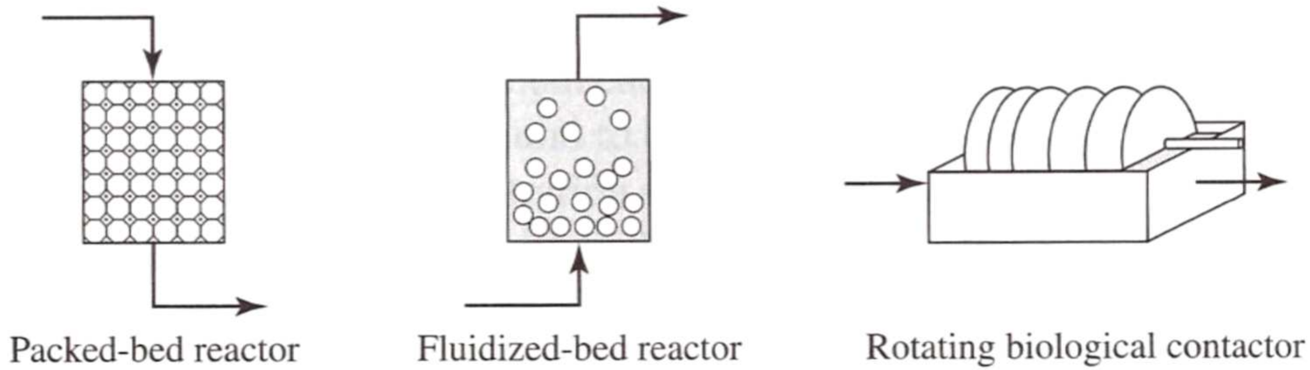
    (with some knowledge buildup for numerical analysis)

Bioreactors

Suspended growth:



Attached growth:



Suspended vs. attached growth

#1

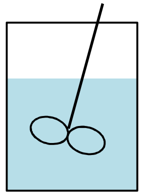
suspended growth

#2

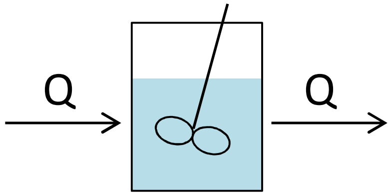
attached growth

Reactors for suspended growth

- **Batch reactor**
  - Bench-scale test systems
  - Some wastewater processes – "sequencing batch reactors"



- **Continuously-stirred tank reactor (CSTR)**
  - Activated sludge
  - Flocculator



- **Plug flow reactor (PFR)**
  - Disinfection
  - Long river/canal
  - Pipeline/aqueduct

Reactor analysis

1. Draw schematics, define control volume, make assumptions if necessary
2. Set mass balance (for a **<u>single</u>** substance!!!)

(mass rate of accumulation)

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

+ (mass rate of gain/loss)

↖

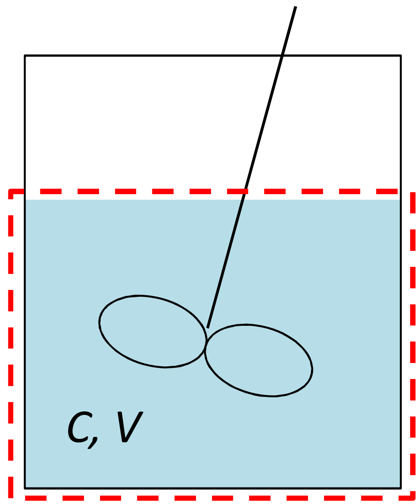
Any processes related to gain/loss, but here we are interested in reactions!

3. Rearrange/solve the equation to a useful form

Reactor analysis: Batch reactor, 1st order

1) Schematics, CV & assumption:

entire reactor as CV, complete mixing, initial concentration = C_0



2) Set mass balance (for the contaminant)

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

3) Rearrange/solve

$$\frac{dC}{C} = -kdt \Rightarrow \int_{C_0}^{C} \frac{dC}{C} = -\int_{0}^{t} kdt \Rightarrow \ln C - \ln C_0 = -kt$$

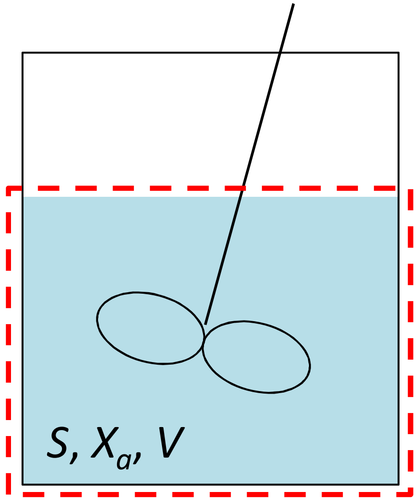
$$\boxed{C/C_0 = e^{-kt}}$$

Reactor analysis: Batch reactor, Monod

1) Schematics, CV & assumption:

initial substrate concentration = S^0

initial active biomass concentration = X_a^0



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, Monod: Governing & initial eqs.

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, Monod: Challenge

Our interest would be *S* vs *t*, X_a vs *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:

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

[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 n^{th} and $n+1^{th}$ time step, the 1^{st} 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 n^{th} 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 $n+1^{th}$ time step

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} ${X_a}^{n+1}$

:

References

#1) https://www.wecprojects.com/media/articles/understanding-activated-sludge-wastewater-management-a-process-overview/

#2) http://www.purewatergazette.net/blog/texas-city-struggles-under-invasion-of-water-filter-flies-june-11-2013/