

Tema 6 – Reactores Reactors

CI7115 – Biotecnología Ambiental

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Conceptos de termodinámica en biotecnología ambiental

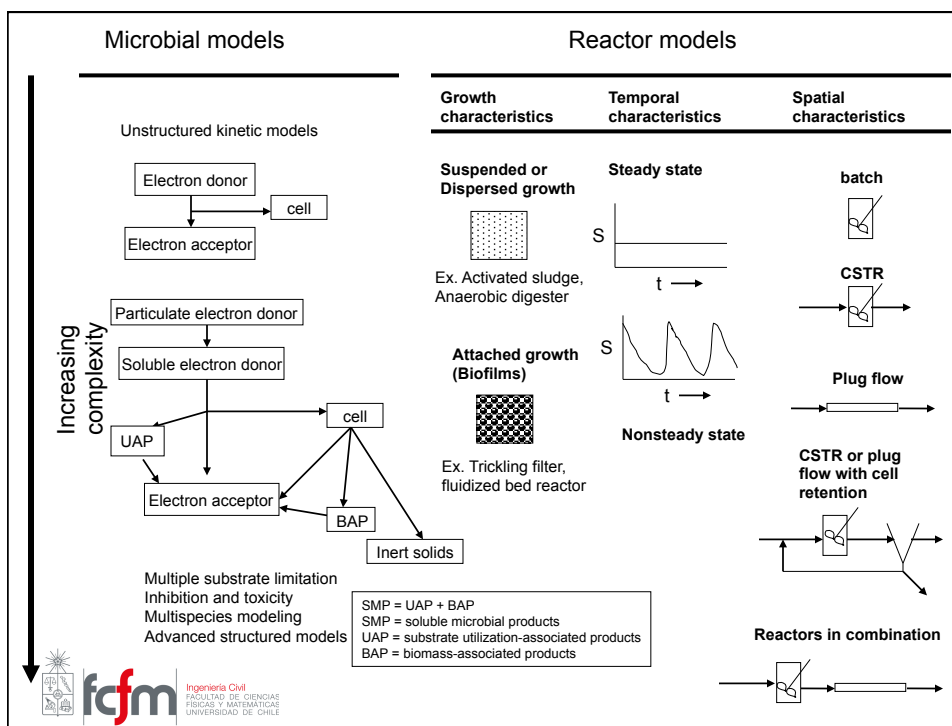
Conservation of Energy - the First Law

- energy balance on a bioreactor (digesters, landfills, compost)
- heat of metabolism
- energy recovery

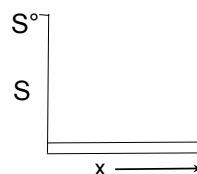
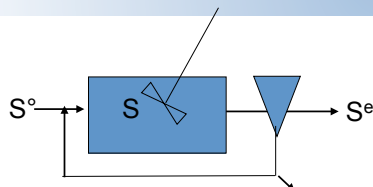
Free Energy - the Second Law

- feasible reactions
- thermodynamic preferences
- relationship between free energy and yield

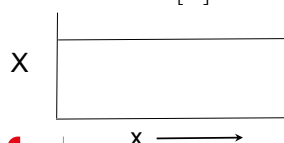




Continuous-flow Stirred Tank Reactor (CSTR)



$$q = \frac{1}{K} \left[\frac{S}{K + S} \right] = \left[\frac{q}{K} \right] S = K_1 S \text{ (for low } S \text{)}$$



Throughout reactor, q is uniform and low because S is low and uniform everywhere.

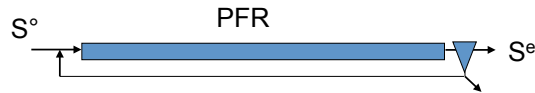
Advantages:

- Resistant to toxics and shock loads because of rapid dilution
- Good for high pH waste where CO_2 provides neutralization
- Good for low pH volatile fatty acid wastes because they are quickly diluted and degraded
- Has spatially uniform oxygen demand.

Disadvantages:

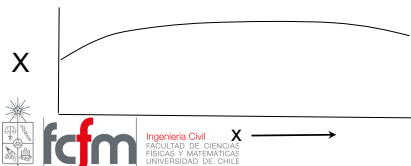
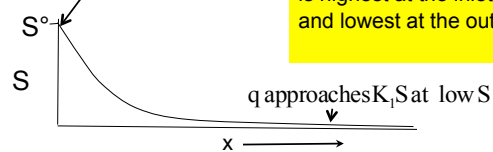
- Less efficient
- Poor settling biomass (filamentous branching) due to uniform low substrate level

Plug Flow Reactors (PFR)



$$q = \hat{q} \left[\frac{S^\circ}{K + S^\circ} \right]$$

approaches \hat{q} at high S°



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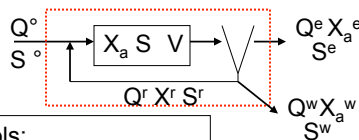
Advantages:

- More efficient
- Variable substrate levels select for better settling biomass

Disadvantages:

- Can be more sensitive to toxics and shock loads because there is less dilution at the reactor entrance
- Oxygen demand is not uniform

Dispersed Growth - CSTR ± recycle



Symbols:

Q - flowrate (m³/d)
X - suspended solids concentration (i.e., biomass, mg/L = g/m³)
S - substrate concentration, mg/L = g/m³
V - reactor volume, m³

Superscripts - location

e = effluent
° = influent
r = recycle
w = waste

Subscripts - type of suspended solids X

a = active organisms (organic)
i = inert biomass (organic)
in = inorganic suspended solids

Assumptions:

1. Completely mixed (CSTR)
2. Soluble substrate
3. X_a in settling tank = 0 (no storage of solids outside of the reactor)
4. Q° , S° do not vary with time.
5. V is constant.

For a batch system (no flow), a mass balance on substrate gives

In: 0
Out: 0
Source: 0
Sink: $qX_a V_L \Delta t$

$$\Delta M = -qX_a V_L \Delta t \quad (\text{constant liquid volume})$$

For a nonvolatile substrate: $\Delta M/V_L = \Delta S$

$$\frac{-dS}{dt} = qX_a \quad \frac{-dS}{dt} = \frac{\hat{q}SX_a}{K+S}$$

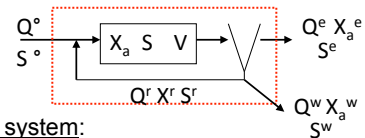
A mass balance on biomass gives

$$\frac{dX_a}{dt} = Y \left(\frac{-dS}{dt} \right) \quad X_a = X_{a0} + Y(S_0 - S)$$

$$t = -\frac{1}{q} \left[\frac{-K}{X_{a0} + YS_0} - \frac{1}{Y} \right] \ln[X_{a0} + YS_0 - YS] + \left[\frac{K}{X_{a0} + YS_0} \right] \ln \left[\frac{SX_{a0}}{S_0} \right] + \frac{1}{Y} \ln X_{a0}$$



For a CSTR (completely mixed with flow)



Mass balance on X_a over ΔT for entire system:

in: 0
out: $(X_a^e Q^e + X_a^w Q^w) \Delta t$
source: $\left(\frac{Y \hat{q} S X_a}{K + S} \right) V \Delta t$ growth ($\mu = Yq$)
sink: $b X_a V \Delta t$ decay

Accumulation = in - out + source - sink

$$V \Delta X_a = 0 - (Q^e X_a^e + Q^w X_a^w) \Delta t + \left(\frac{Y \hat{q} S X_a}{K + S} \right) V \Delta t - b X_a V \Delta t$$



Now Divide by $V \Delta t$

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

Define the **solids retention time** θ_x (also called mean cell residence time, solids residence time, sludge age) where:

$$\theta_x = \frac{V X_a}{(Q^e X_a^e + Q^w X_a^w)} = \frac{\text{mass of active bacteria}}{\text{rate at which active bacteria are removed from system}}$$

Note that θ_x has units of days. It represents the average time solids remain in the system.

At steady state: $\frac{dX_a}{dt} = 0$

Note that θ_x is equal to $1/\mu$. What does that mean?

So the mass balance becomes: $\frac{(Q^e X_a^e + Q^w X_a^w)}{V X_a} = \left(\frac{Y \hat{q} S}{K + S} \right) - b$

$$\text{or } \frac{1}{\theta_x} = \left(\frac{Y \hat{q} S}{K + S} \right) - b$$



Solving for S:

$$S = \frac{K(1 + b\theta_x)}{\theta_x(Y\hat{q} - b) - 1}$$

For soluble substrate, with no substrate utilization in the settling tank, $S^e = S$.

$$\text{Efficiency of substrate utilization: } E = 100 \left(\frac{S^o - S}{S^o} \right)$$

$$\text{For } S \rightarrow \infty, \frac{1}{\theta_x} = \frac{1}{[\theta_x^{\min}]_{\text{lim}}} = Y\hat{q} - b$$

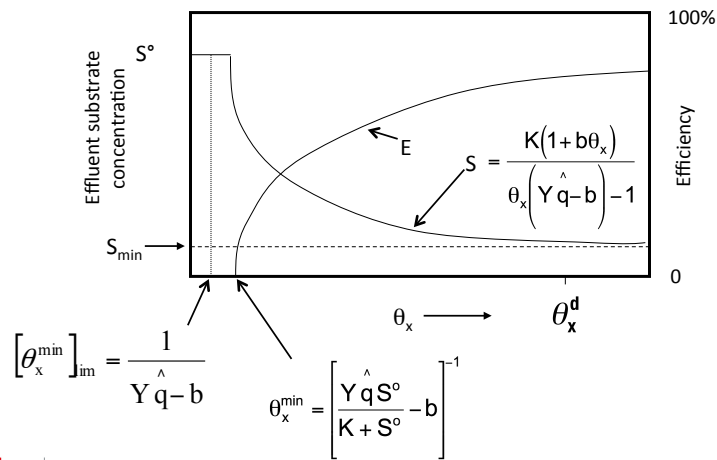
$$\text{For } S = S^o, \frac{1}{\theta_x} = \frac{1}{\theta_x^{\min}} = \frac{Y\hat{q}S^o}{K + S^o} - b$$

If $\theta_x < \theta_x^{\min}$, organism washout occurs



Requirements for biological treatment:

1. Efficiency
2. Reliability



Below which washout occurs

Safety Factor

Design for reliability - safety factor concept:

$$\theta_x^d = S.F. \cdot (\theta_x^{min})_{lim}$$

<u>Loading classification</u>	<u>Implied safety factor (S.F.)</u>
Conventional loading	20-80
High rate loadings	3-10
Low rate loadings	>100

Factors affecting choice of safety factor:

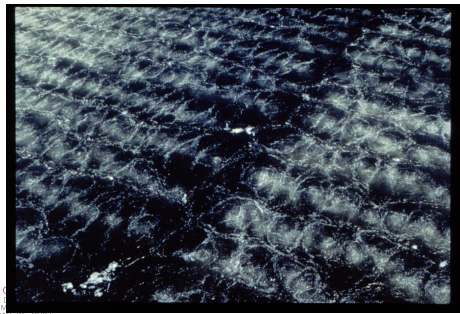
1. Expected temperature variations.
2. Expected wastewater variations (flowrate, organic conc. & composition).
3. Possible presence of inhibitors.
4. Level of operator skill.
5. Efficiency and reliability required.
6. Confidence in design coefficients.

CSTRs with Cell Retention

The above equations are used to model dispersed growth CSTR systems with cell retention.

Applications include:

- Activated sludge (aerobic heterotrophs±nitrifiers)
- Nitrification dispersed growth
- Membrane bioreactors



CSTRs without Cell Retention: $\theta_x = \theta = V/Q^\circ$.

Many systems have no retention of microorganisms. For such systems, $\theta_x = \theta = V/Q^\circ$. The hydraulic residence time equals the solids residence time.

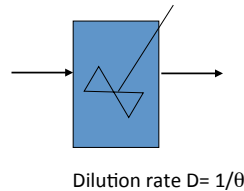
Applications of dispersed growth theory with no cell retention include:

- Chemostats - a useful research tool

- Lagoons



- Digesters

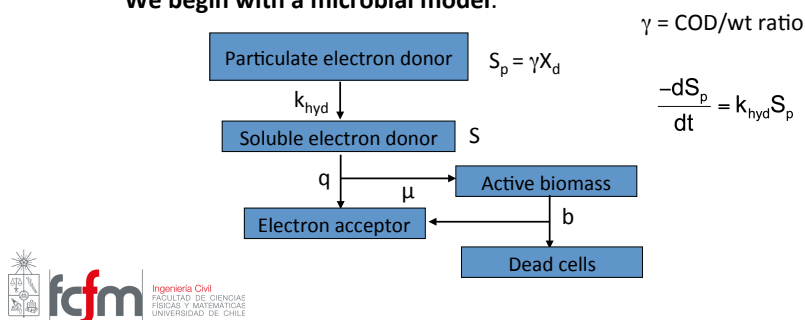


El efecto de los sólidos suspendidos

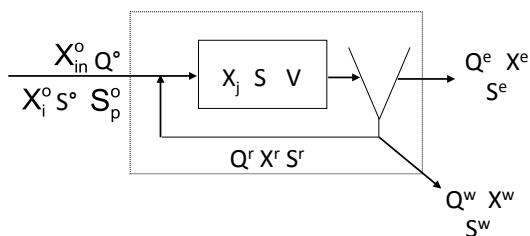
Why do we need a suspended solids balance?

- Biosolids production (amount for further treatment or disposal, nutrient requirements)
- Operational control (effluent quality)
- Reactor design (sizing reactors, choosing the right size aeration equipment)

We begin with a microbial model:



Now we add a reactor model:



Symbols:

Q - flowrate (m^3/d)

X - suspended solids concentration, $\text{mg/L} = \text{g/m}^3$

S - substrate concentration, $\text{mg/L} = \text{g/m}^3$

V - reactor volume, m^3

Superscripts - location

e = effluent

o = influent

r = recycle

w = waste

Subscripts - type of suspended solids X or substrate S

a = active organisms

i = inert organic materials

d = degradable

v = S organics (volatile suspended solids)

in = inorganic

p = particulate

Total suspended solids (TSS) = Mixed Liquor Suspended Solids (MLSS)
 $= X = X_v + X_{in} = \text{volatile} + \text{inorganic}$

Volatile suspended solids (VSS) = Mixed Liquor Volatile Suspended Solids (MLVSS) = $X_v = X_a + X_i + X_d = \text{active} + \text{inert} + \text{biodegradable}$

where:

X_a = active organisms produced from the consumption of soluble substrate S

X_d = biodegradable suspended solids = S_p/γ so that $S_p = \gamma X_d$ where

γ = COD/WT ratio of X_d . (g COD/L = g COD/g VSS x g VSS/L)

Assumptions:

(1) $X_{\text{settling tank}} = 0$

(2) Steady-state operation:

$$\frac{dX_a}{dt} = \frac{dQ^o}{dt} = \frac{dX^o}{dt} = \frac{dS^o}{dt} = \frac{dS_p^o}{dt} = \frac{dQ^e}{dt} = \frac{dX^e}{dt} = \frac{dS^e}{dt} = \frac{dS}{dt} = 0$$

(3) $S^e = S$



Mass balance: change in storage = in - out + source -sink

Consider general suspended solids X_j :

$$V\Delta X_j = \underbrace{Q^o X_j^o}_{\text{in}} \Delta t - \underbrace{(Q^w X_j^w + Q^e X_j^e)}_{\text{out}} \Delta t + (\text{mass production rate}) \Delta t - (\text{mass consumption rate}) \Delta t$$

$$V \frac{dX_j}{dt} = \underbrace{Q^o X_j^o}_{\text{in}} - \underbrace{(Q^w X_j^w + Q^e X_j^e)}_{\text{out}} + \text{mass production rate} - \text{mass consumption rate}$$

At steady state:

$$\underbrace{Q^w X_j^w}_{\text{out}} + \underbrace{Q^e X_j^e}_{\text{in}} = Q^o X_j^o + \text{mass production rate} - \text{mass consumption rate}$$

$$\text{but } \theta_x = \frac{VX_j}{Q^e X_j^e + Q^w X_j^w} \quad (\text{previously determined})$$

$$\text{so } \frac{VX_j}{\theta_x} = Q^w X_j^w + Q^e X_j^e = Q^o X_j^o + \text{mass production rate} - \text{mass consumption rate}$$



and $\frac{VX_j}{\theta_x}$ is the mass removal rate of X_j

(i.e., outflow from the system)

Mass / Time

Assumption:

All of the different types of suspended solids have the same solids retention time.

$$(\theta_x)_{S_p} = (\theta_x)_{X_a} = (\theta_x)_{X_i} = (\theta_x)_{X_{in}} = \theta_x$$

Consider each of the different types of suspended solids in the reactor at steady state:

X_{in} - inorganic suspended solids:

$$Q^o X_{in}^o = \frac{X_{in} V}{\theta_x} \quad \text{but } \frac{V}{Q^o} = \theta$$

$$X_{in} = \frac{\theta_x}{\theta} X_{in}^o$$

θ_x/θ is a kind of concentrating factor



For X_{in} , there is no production and no removal within the reactor (conservative)

S_p or X_d - particulate biodegradable COD ($S_p = \gamma X_d$)

(g COD/L = g COD/g VSS x g VSS/L)

Assume a first order hydrolysis: $\frac{-dS_p}{dt} = k_{hyd} S_p$

$$Q^o S_p^o + 0 - k_{hyd} S_p V = \frac{S_p V}{\theta_x}$$

$$S_p V \left(\frac{1}{\theta_x} + k_{hyd} \right) = Q^o S_p^o$$

$$\frac{S_p (1 + k_{hyd} \theta_x)}{\theta_x} = \frac{S_p^o}{\theta} \quad \text{so} \quad S_p = \frac{\theta_x}{\theta} \frac{S_p^o}{(1 + k_{hyd} \theta_x)}$$



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Dividing both sides by γ :

$$X_d = \frac{\theta_x}{\theta} \frac{X_d^o}{(1 + k_{hyd} \theta_x)}$$

We also note that a mass balance on soluble substrate gives:

$$\begin{aligned} 0 &= Q^o(S^o - S) - qX_a V + k_{hyd} S_p V \\ 0 &= S^o - S - qX_a \theta + k_{hyd} S_p \theta \end{aligned}$$

Substituting in the expression for S_p , we obtain:

$$S_p = \frac{\theta_x}{\theta} \frac{S_p^o}{(1 + k_{hyd} \theta_x)}$$

$$0 = S^o - S - qX_a \theta + k_{hyd} \theta_x \left(\frac{S_p^o}{1 + k_{hyd} \theta_x} \right)$$

In the absence of particulate substrate ($S_p=0$), we have: $0 = S^o - S - qX_a \theta$

Comparing the previous two equations, we see that hydrolysis of particulate substrate effectively increases S^o . We can define an effective influent substrate concentration:

$$S_{eff}^o = S^o + \frac{k_{hyd} \theta_x}{1 + k_{hyd} \theta_x} S_p^o$$

already will be
soluble soluble

S_{eff} is how we account for contribution from particulates



This observation is helpful in preparing a mass balance on active biomass:

X_a - active organisms from soluble substrate S :

$$0 + Y(S_{eff}^o - S^e)Q^o - bX_a V = \frac{X_a V}{\theta_x}$$

$$X_a = \frac{\theta_x}{\theta} \left[\frac{Y(S_{eff}^o - S^e)}{1 + b\theta_x} \right]$$



X_i = inert matter in the influent + dead cells from decay of X_a :

Let f_d = biodegradable fraction of the active cells (~0.8).

Then $1-f_d$ = inert fraction of the active cells (~0.2).

$$\begin{array}{cccc} \text{In} & \text{source} & \text{sink} & \text{out} \\ Q^o X_i^o + (1-f_d)bX_a V - 0 & = & \frac{X_i V}{\theta_x} \end{array}$$

$$X_i = \frac{\theta_x}{\theta} \left[X_i^o + (1-f_d)b\theta_x \frac{Y(S_{eff}^o - S^e)}{1+b\theta_x} \right]$$

$$X_i = \frac{\theta_x}{\theta} \left[X_i^o + (1-f_d)b\theta_x \frac{Y(S_{eff}^o - S^e)}{1+b\theta_x} \right]$$

X_v - volatile suspended solids:

$$X_a = \frac{\theta_x}{\theta} \left[\frac{Y(S_{eff}^o - S^e)}{1+b\theta_x} \right]$$

$$X_v = X_d + X_a + X_i$$

Adding it all up!

$$X_d = \frac{\theta_x}{\theta} \frac{X_d^o}{(1+k_{hyd}\theta_x)}$$

$$X_v = \frac{\theta_x}{\theta} \left[X_i^o + \frac{X_d^o}{1+k_{hyd}\theta_x} + \frac{Y(S_{eff}^o - S^e)(1+(1-f_d)b\theta_x)}{1+b\theta_x} \right]$$

For $f_d = 0.8$,

$$X_v = \frac{\theta_x}{\theta} \left[X_i^o + \frac{X_d^o}{1+k_{hyd}\theta_x} + \frac{Y(S_{eff}^o - S^e)(1+0.2b\theta_x)}{1+b\theta_x} \right]$$

Solids resulting from biological activity:

$$X_{\text{syn}} = X_a + X_{\text{Lsyn}} = \frac{\theta_x}{\theta} \left[\frac{Y(S_{\text{eff}}^0 - S^e)(1 + 0.2b\theta_x)}{1 + b\theta_x} \right]$$

We see that:

$$Y_{\text{eff}} = \frac{Y(1 + 0.2b\theta_x)}{1 + b\theta_x}$$

Because Y is related to f_s :

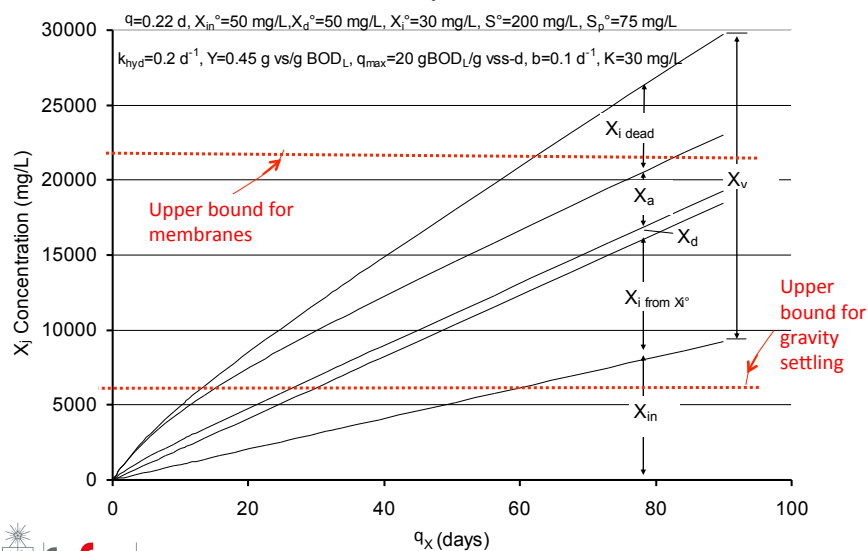
$$f_s = f_s^0 \left(\frac{1 + 0.2b\theta_x}{1 + b\theta_x} \right)$$

For the case with no recycle:

$$Q^w=0, Q^e=Q^0, X^e=X$$

$$\theta_x = \frac{VX_j}{Q^wX_j^w + Q^eX_j^e} = \frac{VX_j^e}{Q^0X_j^e} = \theta$$

Example: change in X_j with q_x for a fixed q



Steady state approach for CSTR design

1. Determine waste characteristics and effluent requirements: Q° , S°_{TOTAL} , S° , S_p° , X_i° , X_{in}° , S°_{max}

where: $S^\circ_{\text{TOTAL}} = \text{BOD}_L$ of the raw waste

$S^\circ = \text{BOD}_L$ of the filtered waste

$S^\circ_{\text{TOTAL}} - S^\circ = S_p^\circ$

X_d° is computed from the COD/WT ratio (γ) for volatile suspended solids.

($X_d^\circ = S_p^\circ / \gamma$)

2. Select coefficients and design factors.

Y , \hat{q} , b , K , S.F., X_v (if cells are retained), k_{hyd} , SMP kinetic parameters
Soluble microbial products



3. Calculate $\left[\theta_x^{\text{min}}\right]_m$. $\left[\theta_x^{\text{min}}\right]_{\text{im}} = \frac{1}{Y \hat{q} - b}$

Apply safety factor

4. Select $\theta_x^d = \text{S.F.} \cdot \left[\theta_x^{\text{min}}\right]_m$.

$$5. \text{ Solve: } S^e = \frac{K(1 + b\theta_x^d)}{\theta_x^d \left(Y \hat{q} - b \right) - 1}$$

If $S^e > S^\circ_{\text{max}}$, increase S.F.



6. Solve for S_{eff}^o .

$$S_{\text{eff}}^o = S^o + \frac{k_{\text{hyd}}\theta_x}{1 + k_{\text{hyd}}\theta_x} S_p^o$$

7. Use the expression:

$$X_v = \frac{\theta_x}{\theta} \left[X_i^o + \frac{X_d^o}{1 + k_{\text{hyd}}\theta_x} + \frac{Y(S_{\text{eff}}^o - S^e)(1 + 0.2b\theta_x)}{1 + b\theta_x} \right]$$

If the reactor has no cell retention:

$$\theta = \theta_x$$



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Solve for X_v .

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7...Continued

If the reactor has cell retention (recycle or membrane):

Solve for θ using the design value for X_v .

Selection of Design X_v :

Gravity settling

Typical settling 1,500- 3,000 mg/L

Poor settling (bulking) 500-1,500 mg/L

Excellent settling (dense) 3,000-5,000 mg/L

Membrane 10,000-20,000 mg/L

8. Solve $V=Q\theta$

Get reactor volume
required



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9. Solve for waste sludge production:

$$X_v \text{ production rate} = \frac{X_v V}{\theta_x^d}$$

$$\text{Remember that } X_{\text{syn}} = X_a + X_i = \frac{\theta_x^d}{\theta} \left[\frac{Y(1 + 0.2b\theta_x^d)(S_{\text{eff}}^o - S^e)}{1 + b\theta_x^d} \right] = \frac{\theta_x^d}{\theta} \left[\overline{X_{\text{syn}}} \right]$$

$$\text{where } \overline{X_{\text{syn}}} = \frac{Y(1 + 0.2b\theta_x^d)(S_{\text{eff}}^o - S)}{1 + b\theta_x^d}$$

$$\text{So the cell production rate is } \frac{(X_{\text{syn}})V}{\theta_x^d} = \left[\frac{V}{\theta_x^d} \right] \left[\frac{\theta_x^d}{\theta} \right] (\overline{X_{\text{syn}}}) = Q^o (\overline{X_{\text{syn}}})$$

Calculation shortcut: it is possible to generalize the above result, as follows:

The production rate (= removal rate) for **ANY** type of suspended solid is equal to $Q^o \overline{X_j}$, where: $\overline{X_j}$ = computed term inside the parentheses of the equation in step 9.



10. Stoichiometry and materials balance:

$$\text{Substrate removal rate} = Q^o (S_{\text{TOTAL}}^o - S^e)$$

$$\text{N requirement} = 0.12 \times \text{Cell production rate (from } C_5H_7O_2N)$$

$$\text{P requirement} = 0.02 \times \text{Cell production rate.}$$

$$\begin{aligned} \text{O}_2 \text{ utilization rate} &= Q^o (S_{\text{eff}}^o - S) - 1.42(\text{cell production rate}) \\ &= Q^o (S_{\text{eff}}^o - S) f_e \\ &= \Sigma \text{O}_2 \text{ equivalent input} - \Sigma \text{O}_2 \text{ equivalent output (biomass)} \end{aligned}$$

Note: the value of S_p^e depends upon the removal efficiency of the separation device. $S_p^e = \gamma (X_d/X_v) X_v^e$, where X_v^e is obtained from a knowledge of clarifier performance and $X_d = (\theta_x^d/\theta) [X_d^o/(1 + k_{\text{hyd}}\theta_x^d)]$.



Table 5.2 Summary of applicable equations for a CSTR with settling and recycle of microorganisms (operating at steady state, treating a soluble substrate, and with no input of active biomass)

Hydraulic Detention Time (θ):

$$\theta = \frac{V}{Q^0} \quad [3.20]$$

Solids Retention Time, SRT (θ_x):

$$\theta_x = \frac{X_a V}{X_a^e Q^e + X_a^w Q^w} \quad [5.35]$$

SRT at which microorganism washout results (θ_x^{\min}), and the limit thereto:

$$\theta_x^{\min} = \frac{K + S^0}{S^0(Y\hat{q} - b) - Kb} \quad S \rightarrow S^0 \quad [3.26]$$

$$\left[\theta_x^{\min}\right]_{\lim} = \frac{1}{Y\hat{q} - b} \quad S \rightarrow \infty \quad [3.27]$$

Reactor or Effluent Substrate Concentration ($S = S^e$):

$$S = K \frac{1 + b\theta_x}{\theta_x(Y\hat{q} - b) - 1} \quad [5.39]$$

Reactor Minimum Substrate Concentration (S_{\min}):

$$S_{\min} = K \frac{b}{Y\hat{q} - b} \quad \theta_x \rightarrow \infty \quad [3.28]$$



Reactor Minimum Substrate Concentration (S_{\min}):

$$S_{\min} = K \frac{b}{Y\hat{q} - b} \quad \theta_x \rightarrow \infty \quad [3.28]$$

Reactor Active Microorganism Concentration (X_a):

$$X_a = \theta_x \frac{X(-r_{ut})}{1 + b\theta_x} \quad [5.40] \quad \begin{aligned} r_{ut} &= q X_a \\ &= -q_{max} S X_a / (K+S) \end{aligned}$$

$$X_a = \frac{\theta_x}{\theta} \frac{Y(S^0 - S)}{1 + b\theta_x} \quad [5.43]$$

Reactor Inert Microorganism Concentration (X_i):

$$X_i = \frac{\theta_x}{\theta} \left[X_i^0 + X_a(1 - f_d)b\theta \right] \quad [5.46]$$

Reactor volatile suspended solids concentration (X_v):

$$X_v = X_i + X_a$$

No particulate substrate,
biodegradable VSS, $X_d = 0$

$$X_v = \frac{\theta_x}{\theta} \left[X_i^0 + \frac{Y(S^0 - S)(1 + (1 - f_d)b\theta_x)}{1 + b\theta_x} \right] \quad [5.47]$$

Active Biological Sludge Production Rate (r_{abp}):

$$r_{abp} = \frac{X_a V}{\theta_x} \quad [5.45]$$

Total Biological Solids Production Rate (r_{tbp}):

$$r_{tbp} = \frac{X_v V}{\theta_x} \quad [5.48]$$

Suspended (dispersed) vs. attached (biofilm) growth

- Suspended (dispersed) growth
 - e.g., Activated sludge, anaerobic digestion
- Attached (biofilm) growth
 - e.g., Trickling filter, fluidized bed reactor

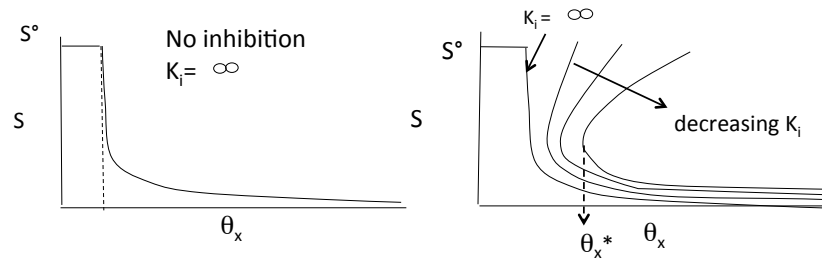
Reactor design for inhibition

For a CSTR, $1/\mu = q_x$

$$\frac{1}{\theta_x} = \mu = Yq - b$$

When there is inhibition, the **expression used for q** depends on the **type of inhibition**.

The Andrews Equation (Haldane kinetics) and its consequence for CSTR treatment (Gaudy et al., 1988)



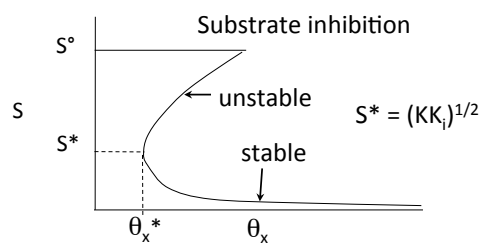
$$\mu = \frac{1}{\theta_x} = Yq - b = \frac{YqS}{K + S + \frac{S^2}{K_i}} - b$$

$$\mu^* = \frac{1}{\theta_x^*} = \frac{Yq}{1 + 2\left(\frac{K}{K_i}\right)^{1/2}} - b$$

Unstable conditions occur when $\theta_x < \theta_x^* = 1/\mu^*$



S should not be allowed to exceed S^*



Design recommendations:

- (1) Pick $\theta_x > \theta_x^*$
- (2) Pick $\theta > \theta_x^*$ to prevent transient loadings from causing $S > S^*$

