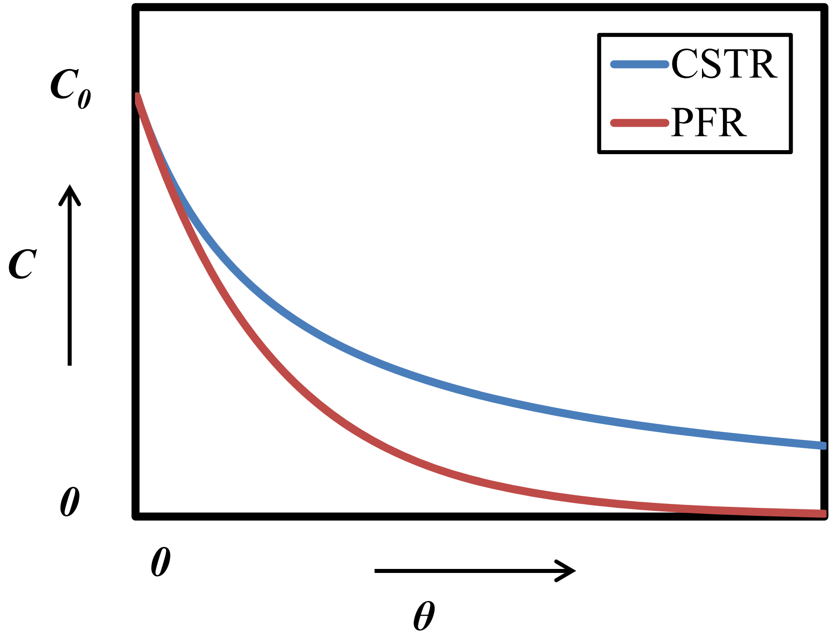
Midterm review II

Reactor analysis

- 1st order reaction $\left.\frac{dC}{dt}\right|_{reaction} = -kC$
  - Batch reactor: $C = C_0 e^{-kt}$
  - PFR: $C = C_0 e^{-k\theta}$
  - CSTR: $C = C_0/(1 + k\theta)$



Reactor analysis

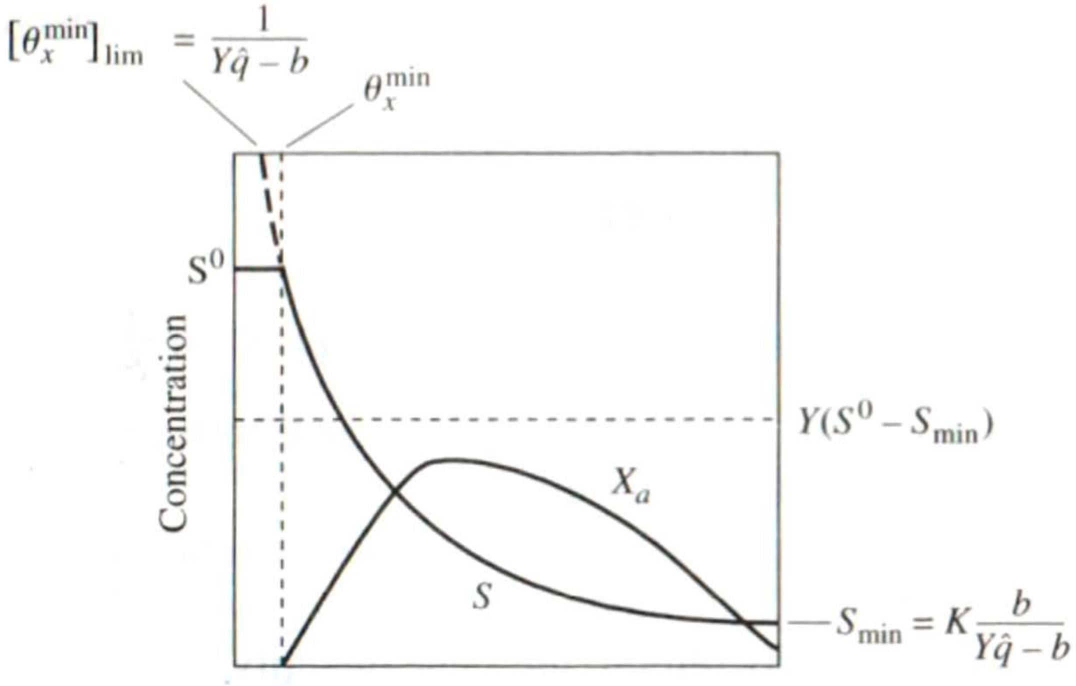
- Monod kinetics

$$\left.\frac{dS}{dt}\right|_{reaction} = r_{ut} = \frac{\hat{q}S}{K+S}X_a$$

$$\left.\frac{dX_a}{dt}\right|_{reaction} = r_{net} = Y\frac{\hat{q}S}{K+S}X_a - bX_a$$

  - Batch reactor: a complicated eq. [5.11] applicable only when decay is negligible
  - PFR: a complicated eq. [5.26] applicable only when decay is negligible
  - CSTR: $S = K\dfrac{1+b\theta}{Y\hat{q}\theta-(1+b\theta)}$ $\quad X_a = Y\dfrac{S^0-S}{1+b\theta}$

Microbial kinetics in a CSTR



1) $\theta_x \leq \theta_{min}$: washout
2) $\theta_x \rightarrow \infty$: $S = S_{min}$
3) For $\theta_{min} < \theta_x$, S decreases with increase in θ_x, but X_a peaks at some point

Microbial kinetics in reactors

Q: Calculate the effluent substrate and active biomass concentration of a bioreactor operated as a CSTR when the influent substrate concentration is 100, 1000, and 10000 mg BOD_L/L. The reactor volume is 1000 m^3 and the flow rate is 250 m^3/hr. Use typical values of Y=0.42 g VSS/g BOD_L, $\hat{q}$=20 g BOD_L/g VSS-d, K=100 mg BOD_L/L and b=0.15 d^{-1} for aerobic degradation of typical organic matter.

Microbial kinetics in a CSTR

- Soluble microbial products
  - Production:

$$r_{UAP} = -k_1 r_{ut} \qquad r_{BAP} = k_w X_a$$

  - Degradation:

$$r_{deg-UAP} = \frac{-\hat{q}_{UAP} UAP}{K_{UAP} + UAP}$$

$$r_{deg-BAP} = \frac{-\hat{q}_{BAP} BAP}{K_{BAP} + BAP}$$

  - Recall a complicated analytical solution in Eqs. [3.38] & [3.39]

Microbial kinetics in a CSTR

- Nutrient consumption

$$r_n = \gamma_n Y r_{ut} \frac{1 + (1 - f_d) b\theta_x}{1 + b\theta_x}$$

$$C_n = C_n{}^0 + r_n \theta$$

- e⁻ acceptor consumption

$$\frac{\Delta S_a}{\Delta t} = \gamma_a Q\left[S^0 - S - SMP + 1.42\left(X_v{}^0 - X_v\right)\right]$$

$$= Q\left[S_a{}^0 - S_a\right] + R_a$$

Microbial kinetics in a CSTR

- Hydrolysis
  - can be reasonably assumed as a 1st-order reaction
  - Then, the result is the increase in "effective" influent substrate concentration

$$r_{hyd} = -k_{hyd} S_p$$

$$S_p = \frac{{S_p}^0}{1 + k_{hyd}\theta}$$

$$S^0{}_{eff} = S^0 + k_{hyd} S_p \theta$$

Microbial kinetics in a CSTR

Q: Compute the effluent COD, BOD$_L$, and NH$_4^+$-N concentration, and the requirement for O$_2$ supply for a chemostat having

$V = 2500\ m^3$

$Q = 10^4\ m^3/d$

$Y = 0.5\ \ g\ \ VSS/g$

$K = 20\ \ mg\ \ COD/L$

$b = 0.15/d$

$\hat{q} = 30\ \ mg\ \ COD/mg\ \ VSS$

$f_d = 0.8$

$X_i{}^0 = X_{in}{}^0 = 50\ \ mg\ \ VSS/L$

$S^0 = 400\ \ mg\ \ COD/L$

$C_N{}^0 = 50\ \ mg\ \ NH_4{}^+ - N/L$

$DO^0 = 8\ \ mg/L$

$DO =\ \ 3\ \ mg/L$

- X_{in} = inorganic VSS

Neglect the production of SMP.

Biofilm kinetics

- Our "idealized" biofilm model:
  - Constant X_f and L_f for the entire biofilm
  - External mass transport described by film theory (Fick's 1st law of diffusion with an "effective diffusion layer")
  - Internal mass transport described by Fick's 2nd law of diffusion
  - Deep vs. shallow biofilm

Biofilm kinetics

- Processes of concern
  - External substrate mass transfer: $J = \frac{D}{L}(S - S_s)$
  - Substrate utilization within biofilm: $r_{ut} = -\frac{\hat{q} X_f S_f}{K + S_f}$
  - Internal substrate mass transfer: $r_{diff} = D_f \frac{d^2 S_f}{dz^2}$
  - Bacterial growth: $\frac{dX_f}{dt} = Y \frac{\hat{q} S_f}{K + S_f} X_f - b' X_f$

Biofilm kinetics

- Governing equations & boundary conditions for substrate mass balance

$$0 = D_f \frac{d^2 S_f}{dz^2} - \frac{\hat{q} X_f S_f}{K + S_f}$$

$$0 = \left.\frac{dS_f}{dz}\right|_{z=L_f} \qquad \frac{D}{L}(S - S_s) = D_f \left.\frac{dS_f}{dz}\right|_{z=0}$$

- Deep biofilm solution: $J_{deep} = \left[2\hat{q} X_f D_f \left(S_s + K\,ln\left(\frac{K}{K + S_s}\right)\right)\right]^{1/2}$

Biofilm kinetics

- Pseudo-steady state assumption: constant X_f and L_f with time

The assumption gives $0 = YJ - b'X_f L_f$

In addition to

$$0 = D_f \frac{d^2 S_f}{dz^2} - \frac{\hat{q} X_f S_f}{K + S_f}$$

$$0 = \left.\frac{dS_f}{dz}\right|_{z=L_f} \qquad \frac{D}{L}(S - S_s) = D_f \left.\frac{dS_f}{dz}\right|_{z=0}$$

Biofilm kinetics

- Pseudo-steady state analytical solution: use non-dimensionalized variables!

1. *Compute the non-dimensional parameters*

$$S^*_{min} = \frac{b'}{Y\hat{q} - b'} \qquad K^* = \frac{D}{L}\left[\frac{K}{\hat{q}X_f D_f}\right]^{1/2} \qquad S^* = \frac{S}{K}$$

2. *Compute α and β*

$$\alpha = 1.5557 - 0.4117\ tanh[log_{10}S^*_{min}]$$

$$\beta = 0.5035 - 0.0257tanh[log_{10}S^*_{min}]$$

Biofilm kinetics

3. *Compute S_s^* (recall our first Excel spreadsheet!)*

$$S_s^* = S^* - J_{deep}^* \cdot f/K^*$$

where $f = tanh\left[\alpha\left(\frac{S_s^*}{S_{min}^*} - 1\right)^{\beta}\right]$

and $J_{deep}^* = (2[S_s^* - ln(1 + S_s^*)])^{1/2}$

4. *Compute J^**

$$J^* = K^*(S^* - S_s^*)$$

5. *Convert J^* to J*

$$J = J^*\left(K\hat{q}X_f D_f\right)^{1/2}$$

6. *Compute $X_f L_f$*

$$X_f L_f = YJ/b'$$

Biofilm kinetics

- Parameter values
  - $\hat{q}, K, Y, and\ b$: obtained from batch experiments
  - D depends on size of a molecule
  - D_f depends on D but is smaller
  - L depends on D and u
  - b' depends on the tangential shear stress

Biofilm kinetics

- Analyzing a completely mixed biofilm reactor
  - Steady state mass balance:

$$0 = QS^0 - QS - J \cdot aV \qquad \text{(substrate)}$$

$$0 = YJ \cdot aV - b'X_f L_f \cdot aV \qquad \text{(active biofilm biomass)}$$

$$0 = -X_a Q + b_{det} X_f L_f \cdot aV \qquad \text{(active suspended biomass)}$$

  - Now *S* as an unknown variable:
    - Iterative approach for *S*: guess *S*, then go through steps 1-6 to get calculated *S*, then guess new *S*, steps 1-6, then …. until guessed *S* = calculated *S*
    - We did this by our second spreadsheet