

Bioreactor analysis & design II

Today's class

- Study on additional variables and analyses
 - Soluble microbial products
 - Nutrient & e⁻ acceptor consumption
 - Hydrolysis

Soluble microbial products (SMP)

- Cell components that released during cell lysis, diffuse through the cell membrane, are lost during synthesis, or are excreted for some purpose
- Does not include intermediates of degradation pathway
- MW = 100s – 1000s
- Biodegradable

Significance of SMP

- Appear in all cases
- Constitute the majority of the effluent COD & BOD in many cases
- Can complex metals, foul membranes, & cause color or foaming

Two types of SMP

- UAP (substrate-**U**tilization-**A**ssociated **P**roducts):
produced directly during substrate metabolism

$$r_{UAP} = -k_1 r_{ut}$$

r_{UAP} = rate of UAP formation [$M_p L^{-3} T^{-1}$]
 k_1 = UAP-formation coefficient [$M_p M_s^{-1}$]

- BAP (**B**iomass-**A**ssociated **P**roducts):
formed directly from biomass as part of
maintenance and decay

$$r_{BAP} = k_2 X_a$$

r_{BAP} = rate of BAP formation [$M_p L^{-3} T^{-1}$]
 k_2 = BAP-formation coefficient [$M_p M_x^{-1} T^{-1}$]

SMP biodegradation

- Assume degradation of both UAP and BAP follow Monod kinetics (with own parameter values for each):

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

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

UAP = concentration of UAP [M_pL⁻³]

BAP = concentration of BAP [M_pL⁻³]

SMP in a CSTR: mass balance

- Steady-state mass balance for UAP & BAP:

$$0 = 0 - Q \cdot UAP - k_1 r_{ut} V - \frac{\hat{q}_{UAP} UAP}{K_{UAP} + UAP} X_a V$$

$$0 = 0 - Q \cdot BAP + k_2 X_a V - \frac{\hat{q}_{BAP} BAP}{K_{BAP} + BAP} X_a V$$

SMP in a CSTR: solutions

$$UAP = -\frac{\hat{q}_{UAP}X_a\theta + K_{UAP} + k_1r_{ut}\theta}{2} + \frac{\sqrt{(\hat{q}_{UAP}X_a\theta + K_{UAP} + k_1r_{ut}\theta)^2 - 4K_{UAP}k_1r_{ut}\theta}}{2}$$

$$BAP = -\frac{K_{BAP} + (\hat{q}_{BAP} - k_2)X_a\theta}{2} + \frac{\sqrt{(K_{BAP} + (\hat{q}_{BAP} - k_2)X_a\theta)^2 + 4K_{BAP}k_2X_a\theta}}{2}$$

Here, the substrate utilization rate, r_{ut} , can be computed by

$$r_{ut} = -\frac{S^0 - S}{\theta} = -\frac{\hat{q}S}{K + S}X_a$$

Observed yield

The VSS in a CSTR is calculated as:

$$X_v = X_i + X_a = X_i^0 + \underbrace{Y(S^0 - S)}_{\text{substrate utilized in the reactor}} \underbrace{\frac{1 + (1 - f_d)b\theta}{1 + b\theta}}_{\text{VSS gained in the reactor}}$$

Influent nbVSS
substrate utilized in the reactor
VSS gained in the reactor

The net yield in the CSTR is: $Y \frac{1 + (1 - f_d)b\theta}{1 + b\theta}$

This value is more often called as **Observed Yield (Y_{obs})**

Nutrient consumption

- For the consumption of nutrients for biomass production:

$$r_n = \gamma_n \cdot Y_{obs} \cdot r_{ut} = \gamma_n \cdot Y \cdot r_{ut} \frac{1 + (1 - f_d)b\theta}{1 + b\theta}$$

r_n = rate of nutrient consumption [$M_n L^{-3} T^{-1}$]

γ_n = the stoichiometric ratio of nutrient mass to VSS for biomass [$M_n M_x^{-1}$]

Using $C_5H_7O_2N$ as cell formula:

$$\gamma_N = 14 \text{ g N} / 113 \text{ g VSS} = 0.124 \text{ g N/g VSS}$$

$$\gamma_P = 0.2 \times 0.124 = 0.025 \text{ g P/g VSS (assume } g P = 0.2 \times g N)$$

Nutrient consumption in a CSTR

- Steady-state mass balance:

$$0 = QC_n^0 - QC_n + r_n V$$

C_n^0 = nutrient conc. in the influent [M_oL^{-3}]

C_n = nutrient conc. in the reactor [M_oL^{-3}]

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

if $C_n < 0$, nutrient-limiting

e⁻ acceptor consumption

(e⁻ acceptor used in a reactor)

= [(total O.D. in the influent) - (total O.D. in the effluent)]
x (conversion factor)

In terms of the use rate for a reactor ($\Delta S_o/\Delta t$):

$$\begin{aligned}\frac{\Delta S_a}{\Delta t} &= \gamma_a [Q(S^0 + 1.42X_v^0) - Q(S + SMP + 1.42X_v)] \\ &= \gamma_a Q [S^0 - S - SMP + 1.42(X_v^0 - X_v)]\end{aligned}$$

γ_a = the stoichiometric ratio of acceptor mass to oxygen demand

for oxygen: 1 g O₂/g COD

for nitrate: 0.35 g NO₃⁻N/g COD

e^- acceptor consumption (cont'd)

To estimate the required mass rate of acceptor supply (ex: aeration $[O_2]$ requirement), the calculated e^- acceptor use rate, $\Delta S_a/\Delta t$ can be written as:

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

$$= \underbrace{Q(S_a^0 - S_a)} + R_a$$

(mass flow rate in) –
(mass flow rate out)

Requirement of e^-
acceptor addition

$[M_a T^{-1}]$

$S_a^0 = e^-$ acceptor conc. in the
influent $[M_a L^{-3}]$

$S_a = e^-$ acceptor conc. in the
reactor $[M_a L^{-3}]$

Hydrolysis of particulates & polymers

- Particulates and polymeric substances account for a significant portion of BOD in wastewater
- >50% of BOD in typical sewage is particulates (SS)
- Particulates and large-MW compounds cannot penetrate the cell membrane
 - needs to be hydrolyzed to smaller molecules
- Catalyzed by extracellular enzymes
- The mechanism and kinetics of hydrolysis is not fully understood

Hydrolysis of particulates & polymers

One simple way of describing hydrolysis is to assume first-order kinetics for particulates (or polymers):

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

r_{hyd} = rate of accumulation of particulates (=dS_p/dt) [M_sL⁻³T⁻¹]

k_{hyd} = first-order hydrolysis rate coefficient [T⁻¹]

S_p = concentration of particulates in the reactor [M_sL⁻³]

In a steady-state CSTR,

$$0 = Q(S_p^0 - S_p) - k_{hyd}S_pV$$

S_p^0 = concentration of particulates in the influent [M_sL⁻³]



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

Hydrolysis of particulates & polymers

- Effect of hydrolysis on dissolved substrates mass balance in a steady-state CSTR

$$0 = Q(S^0 - S) - \frac{\hat{q}S}{K + S}X_aV + k_{hyd}S_pV$$

$$0 = \{(S^0 + k_{hyd}S_p\theta) - S\} - \frac{\hat{q}S}{K + S}X_a\theta$$

→ Increase in S^0 by $k_{hyd}S_p\theta$

→ Increased biomass, but no change in dissolved substrates in the reactor

So: to include the effect of hydrolysis of particulates,

substitute S^0 with $(S^0 + k_{hyd}S_p\theta)$