Reactor analysis

1. Batch reactors

(1) 1st order reaction of a contaminant

1st order reaction: $dC/dt = -kC$

1) define control volume: the entire reactor

2) set mass balance (for the contaminant)

(mass rate of accumulation) = (rate of mass in) – (rate of mass out) + (rate of gain/loss)

$$\frac{dM}{dt} = V\frac{dC}{dt} = 0 - 0 + (-kCV)$$

3) solve the equation

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

* note: don't be confused of dC/dt here and dC/dt when writing reaction kinetics. Here, dC/dt is the change in concentration in the reactor. dC/dt for reaction accounts for the reaction only. If you are confused, add subscripts. Well, for batch reactor, the two should be the same because there's no mass in or out; but for continuous stirred tank reactor, you'll see the difference.

$$\frac{1}{C}dC = -k \cdot dt$$

$$\int_{C_0}^{C} \frac{1}{C}dC = -\int_{0}^{t} k \cdot dt$$

$$\ln C - \ln C_0 = -kt$$

$$\frac{C}{C_0} = e^{-kt}$$

(2) Bacterial growth following Monod kinetics

1) define control volume: the entire reactor (just the same)

2) set mass balance

i) For substrate

$$V\frac{dS}{dt}\bigg|_{reactor} = 0 - 0 + V\frac{dS}{dt}\bigg|_{reaction} = V \cdot r_{ut} = -V\frac{\hat{q}S}{K+S}X_a$$

$$\frac{dS}{dt}\bigg|_{reactor} = -\frac{\hat{q}S}{K+S}X_a$$

ii) For active biomass

$$V\frac{dX_a}{dt}\bigg|_{reactor} = 0 - 0 + V\frac{dX_a}{dt}\bigg|_{net\ growth} = V \cdot \mu X_a$$

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

$$r_{net} = \left(Y\frac{\hat{q}S}{K+S} - b\right)X_a = \mu X_a \text{ , the net rate of active biomass growth } (M_xL^{-3}T^{-1})$$

3) solve the equation

Let's look at the substrate utilization

- this is much more complicated than a simple first order reaction

- the two variables, substrate concentration and active biomass, are intercorrelated

- we have nonlinear forms (not easy to integrate)

[Semi-analytical solution – textbook approach]

Let's assume that decay is negligible (you may find this for growth with relatively efficient e⁻ donors and e⁻acceptors – e.g., aerobic degradation with easily biodegradable organics)

Then, the increase in active biomass is proportional to the substrate utilization with true yield (Y) as a coefficient:

$$X_a = X_a{}^0 + Y \cdot \Delta S = X_a{}^0 + Y\left(S^0 - S\right)$$

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

(still, nonlinear, so you need some engineering math skills to solve this equation – see [5.11])