

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 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

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

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

ii) For active biomass

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

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

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

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)

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:

$$X_a = X_a^0 + Y \cdot \Delta S = X_a^0 + Y(S^0 - S)$$

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

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