Reactor analysis

2. Plug flow reactors

(1) 1st order reaction of a contaminant

1) define control volume: a thin plate perpendicular to the flow

2) set mass balance (for the contaminant)

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

$$\frac{dM}{dt} = \Delta V \frac{dC}{dt} = QC - Q(C + \Delta C) + (-kC\Delta V)$$

At steady state,

$$\frac{dC}{dt} = 0$$

$$0 = -Q\Delta C - kC\Delta V$$

3) solve the equation

$\Delta V = A\Delta z$ (*A*: cross-sectional area)

$$\frac{\Delta C}{\Delta z} = -\frac{k \cdot C \cdot A}{Q}$$

The velocity of the flow within the reactor,

$$u = \frac{Q}{A}$$

$$\frac{\Delta C}{\Delta z} = -\frac{k \cdot C}{u}$$

Now, when $\Delta z \to 0$:

$$\frac{dC}{dz} = -\frac{k \cdot C}{u}$$

$$\frac{1}{C}dC = -\frac{k}{u}dz$$

Integrating z=0 to z,

$$\int_{C_0}^{C}\frac{1}{C}dC = -\int_{0}^{z}\frac{k}{u}dz$$

$$ln\frac{C}{C_0} = -k\cdot\frac{z}{u}$$

At z = L,

$$ln\frac{C_e}{C_0} = -k\cdot\frac{L}{u}$$

The hydraulic retention (detention) time (HRT) in a reactor,

$$\theta = \frac{V}{Q} = \frac{A\cdot L}{A\cdot u} = \frac{L}{u} \qquad [1/T]$$

$$ln\frac{C_e}{C_0} = -k\cdot\theta \qquad \text{(same form as the batch reactor)}$$

(2) Bacterial growth following Monod kinetics

1) define control volume: a thin plate perpendicular to the flow (just the same)

2) set mass balance

i) For substrate

$$\Delta V\frac{\Delta S}{\Delta t} = QS - Q(S+\Delta S) + r_{ut}\cdot\Delta V$$

$$\frac{\Delta S}{\Delta t} = -Q\frac{\Delta S}{\Delta V} + r_{ut}$$

using $u = \frac{Q}{A}$ and $\Delta V = A\Delta z$,

$$\frac{\Delta S}{\Delta t} = -u\frac{\Delta S}{\Delta z} + r_{ut}$$

Now, when $\Delta z \to 0$ and $\Delta t \to 0$:

$$\frac{dS}{dt} = -u\frac{dS}{dz} + r_{ut}$$

At steady state, $dS/dt = 0$

$$u\frac{dS}{dz} = r_{ut} = -\frac{\hat{q}S}{K+S}X_a$$

ii) For active biomass,

$$\Delta V\frac{\Delta X_a}{\Delta t} = QX_a - Q(X_a + \Delta X_a) + \Delta V \cdot \mu X_a$$

$$\Delta V\frac{\Delta X_a}{\Delta t} = -Q\Delta X_a + r_{net}\Delta V$$

Recall that $r_{net} = \left(Y\frac{\hat{q}S}{K+S} - b\right)X_a$ (net rate of active biomass growth)

$$\frac{\Delta X_a}{\Delta t} = -Q\frac{\Delta X_a}{\Delta V} + r_{net}$$

using $u = \frac{Q}{A}$ and $\Delta V = A\Delta z$,

$$\frac{\Delta X_a}{\Delta t} = -u\frac{\Delta X_a}{\Delta z} + r_{net}$$

Now, when $\Delta z \to 0$ and $\Delta t \to 0$:

$$\frac{dX_a}{dt} = -u\frac{dX_a}{dz} + r_{net}$$

At steady state, $dS/dt = 0$

$$u\frac{dX_a}{dz} = r_{net} = \left(Y\frac{\hat{q}S}{K+S} - b\right)X_a$$

* note: You can get the same result by substituting dt with dz/u in the batch reactor solution.

3) solve the equation

According to the correspondence of the batch reactor and the PFR with correlation of dt=dz/u and t=L/u=V/Q=θ (t=batch reactor operation time; L=PFR length; V=PFR volume; Q=PFR flowrate; θ=PFR HRT), you can utilize the batch reactor solutions to easily obtain the PFR solutions.

3. Continuous-stirred tank reactor

(1) 1st order reaction of a contaminant

1) define control volume: the reactor

2) set mass balance (for the contaminant)

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

$$\frac{dM}{dt} = V\frac{dC}{dt} = QC_0 - QC + (-kCV)$$

At steady state,

$$\frac{dC}{dt} = 0$$

$$0 = Q(C_0 - C) - kCV$$

3) solve the equation

$$C = \frac{C_0}{1 + k \cdot V/Q}$$

$V/Q = \theta$, hydraulic retention time – this is an average value for the fluid particles that enter the CSTR! (cf. PFR: all fluid particles have the same HRT)

$$C = \frac{C_0}{1 + k\theta}$$

<u>(2) Bacterial growth following Monod kinetics</u>

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

2) set mass balance

i) For substrate

$$V\frac{dS}{dt} = QS^0 - QS + r_{ut} \cdot V$$

at steady state,

$$0 = QS^0 - QS + r_{ut} \cdot V$$

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

ii) For active biomass,

$$V\frac{dX_a}{dt} = -QX_a + r_{net} \cdot V$$

at steady state,

$$0 = -QX_a + r_{net} \cdot V$$

$$0 = -X_a + \left(Y\frac{\hat{q}S}{K + S} X_a - bX_a \right) \cdot \theta$$

3) solve the equation

With some math:

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

$$X_a = Y\frac{S^0 - S}{1 + b\theta}$$