3.044 Recitation 8
April 7-8, 2005

- Batch/Continuous Flow Reactors
- Flow Through Porous Media

For a first order reaction: $A \rightarrow B$, the reaction might be homogeneous or heterogeneous within different kinds of reactor. Assume that reaction rate k, flow rate , and reactor volume V are the same for all cases.

=Homogeneous Reaction=

Batch Reactor

A batch reactor operates once at a time. It requires extra time (i.e., downtime t_d) for loading and reloading the reactor.

Concervation of Species A:

$$V\frac{dC_A}{dt} = -kVC_A$$

Solving this ODE get

$$C_A = Constant \exp\left(-kt\right)$$

At $t = 0, C_A = C_{A_{initial}}$, thus $Constant = C_{A_{in}}$.

$$\frac{C_A}{C_{A_{in}}} = \exp(-kt)$$

As C_A approaches some small concentration $C_{A,out}$, $t \rightarrow t_R$(residence time:time spent in the reactor). Therefore $t_R = \frac{1}{k}ln(C_{A,in}/C_{A,out})$.

Production rate is $Q = \frac{V}{total\,time} = \frac{V}{t_R+t_d}$.

Continuous Flow Reactor

1. Continuous Stirring Tank Reactor (Perfect Mixing)

Conservation of species A:

$$V\frac{dC_A}{dt} = QC_{A,in} - QC_{A,out} - kVC_A$$

where $C_{A,in}$ is the concentration of A from the inlet flow, $C_{A,out}$ is the concentration of A at the outlet flow, C_A is the concentration of A in the reactor tank. If we assume that there is no accumulation of species A, the concentration of A inside the tank must be equal to the concentration of A coming out from the outlet. So the conservation equation with no accumulation becomes

$$0 = QC_{A,in} - QC_{A,out} - kVC_{A,out}$$

$$(Q + kV)C_{A,out} = QC_{A,in}$$

$$\frac{C_{A,out}}{C_{A,in}} = \frac{Q}{Q+kV} = \frac{1}{1+\frac{kV}{Q}}$$

Production rate is $Q = \frac{kV}{(C_{A,in}/C_{A,out})-1}$.

Testing by tracers: Add some amount of tracers (C_{T_0})inside the tank and measure the flow coming out

$$V\frac{dC_{T,}}{dC_{T_0}} = -QC_T$$

$$ln(C_T) = -\frac{Q}{V}t + constant$$

$$C_t = Constant \exp(-\frac{Qt}{V})$$

At $t = 0$, $C_T = C_{T_0}$ thus $Constant = C_{T_0}$

$$\frac{C_t}{C_{T_0}} = \text{exp(-}\frac{Qt}{V}\text{)}$$

2. Plug Flow Reactor

All species in the reactor have the same residence time $t_R = V/Q$. An ideal PFR acts like a batch reactor.

Conservation of species A:

$$V\frac{dC_A}{dt} = -kVC_A$$

This has the same $C_A(t)$ function as the batch reactor. At $t = t_R$,$C_A = C_{A,out}$. Therefore

$$\frac{C_{A,out}}{C_{A_{in}}} = \text{exp(-}kt_R\text{)} = \text{exp(-}\frac{kV}{Q}\text{)}$$

Production rate: $Q = \frac{kV}{ln(C_{A,in}/C_{A,out})}$.
Testing by tracers: Add some amount of tracers into the reactor and measure the amount that comes out. In this case, tracers will diffuse as they move through the reactor. The diffusion lenght is calculated by

$L_D = \sqrt{Dt}$

After $t = t_R = V/Q$,the diffusion length is L'_D

$L'_D = \sqrt{D\frac{V}{Q}} = \sqrt{Dt_R}$

Dimensionless length can be written as the ratio between reactor length and the diffusion length

$\frac{L}{L'_D} = \sqrt{\frac{L^2}{Dt}} = \sqrt{\frac{UL}{D}} = \sqrt{Pe}$

Pe is Peclet number. It is the ratio of bulk mass transfer and diffusive mass transfer.

=Heterogeous Reaction=

Heterogeneous reaction occurs at the surface. The rate limitting factor is the mass transfer coefficient (h_D) or evaporation reaction rate (k"). We can derive all the above equations for heterogeneous cases by using $h_DA$or k"A instead of kV. In this case, A is the surface area where the reaction occurs.

Flow Thru A Porous Media

List of symbols

k_D :Permeability $[\frac{m^4}{Ns}]$

$\mathcal{P}$: Specific permeability $[m^2]$

$\triangle P'$:Pressure drop and gravity term:$\triangle P' = \triangle P + \rho g L$

V_0 :Superficial velocity $[\frac{m}{s}]$

$\overline{V}$: Avg Velocity of flow through a porous media $[\frac{m}{s}]$

V_h :Volume of pores: Volume of fluid

V_{solid} :Volume of solid

V: Volume of the reactor

A_ω :Wetting area

R_h : Hydraullic radius (Characteristic radius for flow through a porous media) $[m]$

ω : Volume fraction of pores

$1-\omega$:Volume fraction of solid

S_0 :Wetting surface area per unit volme of solid $[\frac{1}{m}]$:$S_0 = \frac{A_\omega}{V_{solid}}$

S :Wetting surface area per unit volume of reactor $[\frac{1}{m}]$: $S = S_0(1-\omega)$

Darcy's law[1] states that if the pressure gradient is low, the flow rate per unit area is proportional to the pressure drop per unit length. The proportional factor is the permeability, k_D and $A$is the total cross-sectional area including pores.

$V_0 = \frac{Q}{A} = k_D \frac{\triangle P'}{L} = \frac{\mathcal{P}}{\mu} \frac{\triangle P}{L}$

Tube-bundle theory takes the Hagen-Pouiseuille equation and states that the average velocity of flow through a bundle of tube is proportional to that through a single tube. The proportional factor is K_1 and the radius is R_h.

$\overline{V} = K_1 \frac{\triangle P' R_h^2}{\mu L}$

Relating V_0 and $\overline{V}$ by setting $V_0 = \overline{V}\omega$ and substituting R_h with ω/S, get

$\mathcal{P} = K_1 \frac{\omega^3}{S^2}$

Reynolds number for flow through a bundle tube is

$Re_c = \frac{\rho U R}{\mu} = \frac{\rho \bar{V} R_h}{\mu} = \frac{\rho \overline{V} \omega}{\mu S} = \frac{\rho V_0}{\mu(1-\omega) S_0}$

Example

Molten aluminum is flown through a horizontal packed bed of alumina spheres with uniform d=0.5cm and the length of the bed is $L = 1m$. The fraction of sphere is 0.61. Given $\rho_{Al} = 2100 \frac{kg}{m^3}$, $\mu = 10^3 \frac{Ns}{m^2}$, and $V_0 = 0.5m/s$

(a) What is S?

$S_0 \approx \frac{\pi d^2}{\frac{\pi}{6} d^3} = \frac{6}{d}$

$S = S_0(1-\omega) = \frac{6}{0.5x10^{-2}}(0.61) = 732\ m^{-1}$

(b) Calculate Re

$Re_c = \frac{\rho V_0}{\mu S} = \frac{2100(0.5)}{10^3(732)} = 0.001$

(c) Calculate pressure gradient ($K_1 = 1/4.2$ for a packed bed of sphere)

$\mathcal{P} = K_1 \frac{\omega^3}{S^2} = \frac{0.39^2}{4.2 * 732^2} = 6.75 \times 10^{-8} m^2$

$\frac{\triangle P}{L} = \frac{V_0 \mu}{\mathcal{P}} = \frac{0.5(10^3)}{6.75 \times 10^{-8}} = 7.4 \times 10^9 \frac{N}{m^3}$

[1] Poirier and Geiger, Section 3.4