10.37 Chemical and Biological Reaction Engineering, Spring 2007
Prof. William H. Green
Lecture 25: Course Review

Review

Fundamental Equations:

Acc = Flow In – Flow Out + Reaction

$$\frac{\partial n_m}{\partial t} = F_{m,o} - F_{m,out} + \iiint r_m(x,y,z,t)dxdydz$$

infinitesimal volume

$$\frac{\partial C_m}{\partial t} = \nabla \cdot F_m + r_m$$

$K_{eq} = e^{-\Delta G_{rxn}/RT}$ (K_{eq} is unitless)

$$K_{eq} = \frac{\prod_{m=1}^{\text{N products}} \left(P_m / 1\ bar \right)^{\nu_n}}{\prod_{j=1}^{\text{reactants}} \left(P_j / 1\ bar \right)^{-\nu_j}}$$

$$K_c = \frac{k_{forward}}{k_{reverse}}$$

$$H_2O_2 \rightarrow H_2 + O_2$$

$$\frac{n}{V} = \frac{P}{RT}$$

$$K_{eq} = \frac{\left(P_{H_2} / 1\ bar \right)\left(P_{O_2} / 1\ bar \right)}{\left(P_{H_2O_2} / 1\ bar \right)}$$

$$K_c = \frac{[H_2][O_2]}{[H_2O_2]}$$

units $K_c [=] \frac{mol}{L}$

Convection dominated:

Constant P, constant T, constant reactor V

$$F_m \approx \nu C_m$$

$$\nabla \cdot W_m \approx D\nabla^2 C_m + \vec{U} \cdot \vec{\nabla} C_m$$

Pressure drop in Packed Bed:

Ergun Equation: $$\frac{\partial P}{\partial z} = -\frac{G}{pg_c D_p}\frac{1-\phi}{\phi^3}\left[\frac{150(1-\phi)\mu}{D_p} + 1.75G\right]$$

$$\frac{\partial U_{cv}^{tot}}{\partial t} + P\frac{\partial V_{cv}}{\partial t} = \sum F_j \bar{H}_j + \dot{Q} + \dot{W}_s$$ (U_{cv}^{tot} depends on T)

$$\frac{\partial T}{\partial t} = \left\{\frac{\nu\tilde{C}(T_{in} - T_{out}) + \dot{Q} + \sum r_k \Delta H_{rxn}}{C_{total}}\right\}$$ where $\tilde{C}$ is the heat capacity

Special Cases:

Perfectly Homogeneous ("well stirred", "perfectly mixed")

→ no flows, "batch reactor"

$$\frac{\partial n_m}{\partial t} = r_m\left(\underline{C}(t)\right)V$$

→ CSTR, no t-dependence

$$0 = F_{in} - F_{out} + r\left(\underline{C}_{out}\right)$$

Homogeneous in x,y, not in z (no t-dependence)

PFR (typically gives higher productivity than CSTR)

$$\frac{\partial F_m}{\partial z} = Ar_m\left(\underline{C}(z)\right)$$

"sort of" PFR

$$\frac{\partial F_m}{\partial z} = Ar_m\left(\underline{C}^{avg}(z)\right)\Omega(z)$$ where $\Omega(z)$ is the effectiveness factor

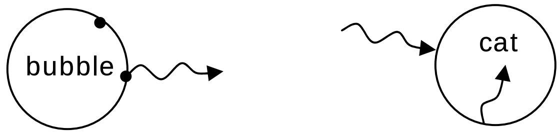

Figure 1. a) mass transfer from gas to liquid b) mass transfer into catalyst particle

$$D\frac{\partial^2 C_m}{\partial r^2}+\left(\frac{2}{r}\right)\frac{\partial C_m}{\partial r}+r_m\left(\underline{C}(\underline{r})\right)=0$$

- nondimensionalize
- some solutions in book
- (18.03)

guess solution, plug in to verify
matlab

Thiele modulus

$$\phi^2 \equiv \frac{r_m\left(\underline{C}_{surface}\right)}{D_{solid}\, C_{m,s}/R^2}$$

- if small (<1): reaction limited, ignore effectiveness factor Ω (internal diffusion fast)
- if big: transport matters!

$$F_{\substack{from\\bubble}} = Ak_L(C_{interface}-C_{bulk})$$

$k_L A$ → correlations
(sphere-packed bed)

$$F_{\substack{into\\particle}} = k_c A(C_{bulk}-C_s) \qquad k_c \sim \frac{D}{\delta}$$

Converting the second-order differential equation into first-order ordinary differential equations for MatLab solvers:

$$\frac{\partial C_m}{\partial r}=q_m$$

$$D\frac{\partial q_m}{\partial r}+\frac{2}{r}q_m+r_m=0$$

→ $\frac{\partial q_m}{\partial r}=\frac{-\frac{2}{r}q_m+r_m}{D}$ → MATLAB: ode15s