ChE 344 Winter 2016: Final exam equation sheet
Dr Trent Silbaugh, Instructor

Fundamental Equation

$$\frac{dN_A}{dt} = F_{A0} - F_A + \int^V r_A dV$$

Design Equations

	Conversion Basis		Molar Basis	
Batch	$N_{A0}\frac{dX}{dt} = -r_A V$	$t_1 = N_{A0}\int_0^X \frac{dX}{-r_A V}$	$\frac{dN_A}{dt} = r_A V$	$t_1 = \int_{N_{A_1}}^{N_{A_0}} \frac{dN_A}{-r_A V}$
CSTR	$V = \frac{F_{A0}(X_{out} - X_{in})}{-r_{A_{out}}}$		$V = \frac{F_{Ain} - F_{Aout}}{-r_{A_{out}}}$	
PFR	$F_{A0}\frac{dX}{dV} = -r_A$	$V_1 = F_{A0}\int_{X_{in}}^{X_{out}} \frac{dX}{-r_A}$	$\frac{dF_A}{dV} = r_A$	$V_1 = \int_{F_{A_1}}^{F_{A_0}} \frac{dF_A}{-r_A}$
PBR	$F_{A0}\frac{dX}{dW} = -r_A'$	$W_1 = F_{A0}\int_{X_{in}}^{X_{out}} \frac{dX}{-r'_A}$	$\frac{dF_A}{dW} = r_A'$	$W_1 = \int_{F_{A_1}}^{F_{A_0}} \frac{dF_A}{-r'_A}$

Ideal gas law: $pV = nRT$ $\qquad R = 8.314\frac{J}{mol.K} = 1.987\frac{cal}{mol.K}$

Arrhenius Equation: $k_A(T) = A\cdot\exp\left[\frac{E_A}{-RT}\right]$ $\qquad k_A(T) = k_A(T_0)\cdot\exp\left[\frac{E_A}{R}\left(\frac{1}{T_0} - \frac{1}{T}\right)\right]$

$$K_C(T) = K_C(T_0)\cdot\exp\left[\frac{\Delta H^o_{rxn}}{R}\left(\frac{1}{T_0} - \frac{1}{T}\right)\right]$$

Stoichiometry:

For Reaction: $aA + bB \to cC + dD$ Liquid Phase: $C_i = C_{A0}(\Theta_i - v_i X)$

Gas Phase: $C_i = \frac{C_{A0}(\Theta_i + v_i X)}{1+\varepsilon X}\left(\frac{P}{P_0}\right)\left(\frac{T_0}{T}\right)$ $\qquad v = v_0(1+\varepsilon X)\left(\frac{T}{T_0}\right)\left(\frac{P_0}{P}\right)$

$$\Theta_i = \frac{F_{i0}}{F_{A0}} = \frac{C_{i0}}{C_{A0}} = \frac{y_{i0}}{y_{A0}} \qquad \delta = \frac{d}{a} + \frac{c}{a} - \frac{b}{a} - 1 \qquad \varepsilon = y_{A0}\delta$$

Packed Beds:

laminar turbulent

$$\frac{dP}{dz} = -\frac{G}{\rho g_c D_P}\left(\frac{1-\phi}{\phi^3}\right)\left[\frac{150(1-\phi)\mu}{D_P} + 1.75G\right] \qquad \frac{dP}{dW} = -\frac{\alpha}{2}\frac{P_0}{P/P_0}\left(\frac{T}{T_0}\right)(1 + y_{A0}\delta X)$$

$$\beta_0 = -\frac{G}{\rho_0 g_c D_P}\left(\frac{1-\phi}{\phi^3}\right)\left[\frac{150(1-\phi)\mu}{D_P} + 1.75G\right] \qquad \alpha = \frac{2\beta_0}{A_C\rho_c(1-\phi)P_0} \qquad dW = (1-\phi)A_C\rho_c\,dz$$

If isothermal and $\delta = 0$ or X is very small: $\frac{P}{P_0} = (1 - \alpha W)^{1/2}$

Energy Balance

$$\frac{d\hat{E}_{sys}}{dt} = \dot{Q} - \dot{W}_s + \sum F_i H_i\Big|_{in} - \sum F_i H_i\Big|_{out}$$

For Steady State System in Single Phase
$0 = \dot{Q} - \dot{W}_s - F_{A0}\sum_{i=1}^{n}\Theta_i\overline{C_{P_i}}(T - T_{i0}) - \Delta H_{Rx}(T)F_{A0}X$ where $H_{Rx}(T) = \Delta H_{Rx}^o(T_R) + \underbrace{\Delta C_p}_{\sum \nu_i C_{Pi}}(T - T_R)$

Adiabatic System (CSTR, PFR, PBR, Batch)
Conversion $X = \dfrac{\Sigma\Theta_i C_{P_i}(T - T_0)}{-[\Delta H_{Rx}^\circ(T_R) + \Delta C_P(T - T_R)]}$
Temperature $T = \dfrac{X[-\Delta H_{Rx}^\circ(T_R)] + \Sigma\Theta_i C_{P_i}T_0 + X\Delta C_P T_R}{\Sigma\Theta_i C_{P_i} + X\Delta C_P}$

PFR with heat exchange

$$\frac{dT}{dV} = \frac{\overbrace{r_A\Delta H_{Rx}}^{\substack{Q_g \\ Heat\ "Generated"}} - \overbrace{Ua(T - T_a)}^{\substack{Q_r \\ Heat\ "Removed"}}}{\Sigma F_i C_{P_i}}$$

Unsteady State CSTR and Semibatch

$$\frac{dT}{dt} = \frac{\dot{Q} - \dot{W}_s - \sum F_{i0}\overline{C_{P_i}}(T - T_0) + (-\Delta H_{Rx})(-r_A V)}{\Sigma N_i C_{P_i}}$$

Multiple Reactions:
Selectivity and Yield

Instantaneous Selectivity	$S_{D/U} = {r_D}/{r_U}$
Overall Selectivity	$\tilde{S}_{D/U} = {F_D}/{F_U}$
Instantaneous Yield	$Y_{D/A} = {r_D}/{-r_A}$
Overall Yield	$\tilde{Y}_{D/U} = {F_D}/{F_{A0} - F_A}$

External and Internal Diffusion:

$$W_{AZ} = k_c(C_{AB} - C_{AS})$$

$$System\ with\ reaction\ only\ on\ external\ surface\ area{:}\ C_{AS} = \frac{k_c}{k" + k_c}C_{AB}$$

$$Re = \frac{\rho U d_p}{\mu} \qquad Sh = \frac{k_c d_p}{D_{AB}} \qquad Sc = \frac{\nu}{D_{AB}}$$

Correlation for flow around a sphere: $Sh = 2 + 0.6Re^{1/2}Sc^{1/3}$

$$\eta = \frac{r_{obs}}{r_{max}} = \frac{\tanh(\phi_1)}{\phi_1}, \phi_1 = L_P\sqrt{\frac{k}{D_{AB}^e}}\ \ where\ \ D_{AB}^e = \frac{D_{AB}\phi_p\sigma_c}{\tilde{\tau}}$$

$$and\ \ L_P = x_P\ (slab),\ \frac{R_P}{3}\ (sphere),\ \frac{R_P}{2}(cylinder)$$

Enzyme Kinetics:

ChE 344 Winter 2016: Final exam equation sheet
Dr Trent Silbaugh, Instructor

$$Michaelis - Menten\ Equation: r_{product} = \frac{V_{max}[S]}{K_M + [S]}$$

Lineweaver-Burke Analysis: $\frac{1}{r_p}\ versus\ \frac{1}{[S]}$

Integrals:

$$\int_0^X x^a dx = \frac{x^{a+1}}{a+1}, \qquad a \neq -1$$

$$\int_0^X \frac{dX}{1+\varepsilon X} = \frac{1}{\varepsilon}\ln(1+\varepsilon X)$$

$$\int_0^X x^{-1} dx = \ln(x)$$

$$\int_0^X \frac{1+\varepsilon X}{1-X} dX = (1+\varepsilon)\ln\left(\frac{1}{1-X}\right) - \varepsilon X$$

$$\int_0^X \frac{dX}{1-X} = \ln\left(\frac{1}{1-X}\right)$$

$$\int_0^X \frac{1+\varepsilon X}{(1-X)^2} dX = \frac{(1+\varepsilon)X}{1-X} - \varepsilon\ln\left(\frac{1}{1-X}\right)$$

$$\int_0^X \frac{dX}{(1-X)^2} = \frac{X}{1-X}$$

$$\int_0^W (1-\alpha W)^{1/2} dW = \frac{2}{3\alpha}\left[1-(1-\alpha W)^{3/2}\right]$$

$$\int_0^X \frac{(1+\varepsilon X)^2}{(1-X)^2} dX = 2\varepsilon(1+\varepsilon)\ln(1-X) + \varepsilon^2 X + \frac{(1+\varepsilon)^2 X}{1-X}$$

$$\int_0^X \frac{dX}{(1-X)(\Theta_B - X)} = \frac{1}{\Theta_B - 1}\ln\left(\frac{\Theta_B - X}{\Theta_B(1-X)}\right), \qquad \Theta_B \neq 1$$

$$\frac{dy}{dt} + P(t)y = Q(t), \qquad I(t) = e^{\int P(t)}, \qquad \frac{d\big(yI(t)\big)}{dt} = Q(t)I(t), \qquad y = \frac{1}{I(t)}\int Q(t)I(t)dt$$

Roots for: $ax^2 + bx + c \qquad \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$