10.37 Chemical and Biological Reaction Engineering, Spring 2007
Prof. William H. Green
Lecture 6: Concentration that Optimizes a Desired Rate

This lecture covers: Selectivity vs. conversion and combining reactors with separations.

Optimal

- What is the target? goal? → Often it is to maximize profit or production

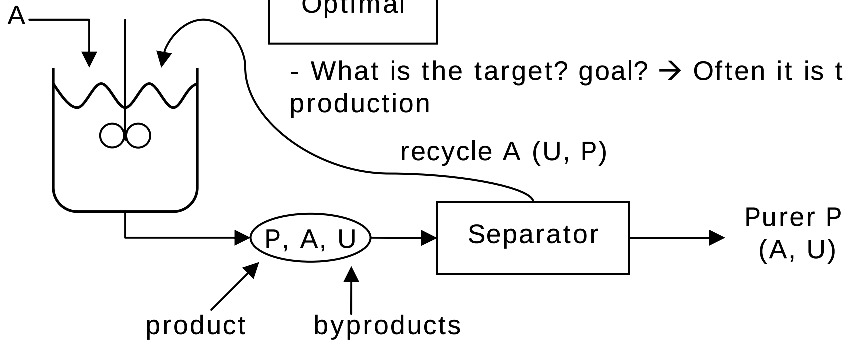

Figure 1. Schematic of a reacting system with a recycle stream.

Simple Target: maximize $F_p = r_p \cdot \underbrace{V}_{\text{const. (vol.)}}$

r_p (concentrations, T)

Constraint: $T \le T_{\max}$
High temperature → maximum rate constant

Simplest Case:

$A \rightarrow P \qquad r_p = k[A] \qquad [A] \Rightarrow [A]_{feed}$

$\tau \rightarrow 0$
residence time in reaction

$$F_p = [P]V_0 = [P]\frac{V}{\tau}$$

$$= Vk[A]_{feed}\frac{(1-e^{-Da})}{Da}$$

Constraint: $[P] \ge [P]_{\min}$ (purity constraint)
→ $X \ge X_{\min}$ conversion

$$F_p = k(T_{\max})\left\{[A]_0 - [P]_{\min}\right\}V = k(T_{\max})[A]_{feed}V(1-X)$$

$A + B \rightarrow 2C$ 2nd order

$r_c = 2k[A][B]$

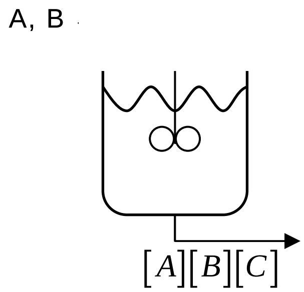

Figure 2. Schematic of a CSTR.

$$[A] = [A]_{feed}(1 - X_A)$$

$$[B] = [B]_{feed}(1 - X_B)$$

$$r_c = 2k[A]_{feed}[B]_{feed}(1 - \overset{.1}{X_A})(1 - \overset{.1}{X_B})$$

.01

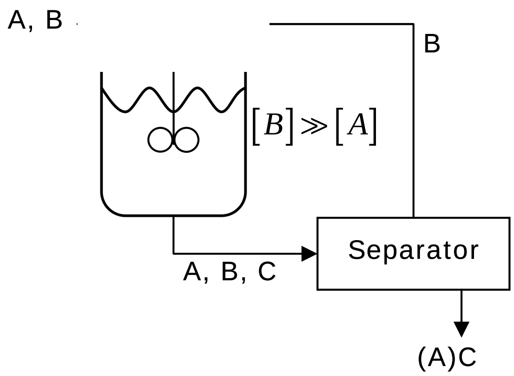

Figure 3. A reacting system with recycle stream.

$A \rightarrow \boxed{B}$ product may also react

$B \rightarrow C$

$A \rightarrow U$ undesirable

$F_B = f([A],[B],[C],[U],\tau,T)$

6 variables

→ fsolve (Matlab)

SS. $0 = F_{\underset{A}{in}} - F_{\underset{A}{out}} + r_A V$

$0 = F_{\underset{B}{in}} - F_{\underset{B}{out}} + r_B V$

$0 = \ldots$

$0 = \ldots$

Simplest Case:

$$A \xrightarrow{k_1(T)} B$$

$$B \xrightarrow{k_2(T)} C$$

$$A \xrightarrow{k_3(T)} U$$

$$[A] = \frac{F_{A_{in}}}{V(k_1 + k_3 + 1/\tau)}$$

$$[U] = k_3 [A] \tau$$

$$[C] = k_2 \tau [B]$$

$$[B] = \frac{k_1 [A]}{k_2 + \frac{1}{\tau}}$$

$$\boxed{F_B(\tau, T)} = \frac{F_{Ao}\underbrace{k_1\tau}_{D_{a_1}}}{(\underbrace{k_1\tau}_{D_{a_1}} + \underbrace{k_3\tau}_{D_{a_2}} + 1)(1 + \underbrace{k_2\tau}_{D_{a_3}})}$$

optimize
2 variables
→ contour plot

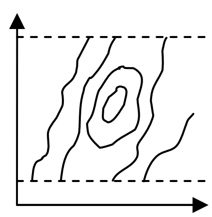

Figure 4. Sample contour plot for the 2-variable optimization.

matlab→fmincon
(allows for constraints)

$$\underbrace{\frac{\partial F_B}{\partial T} = 0, \ \frac{\partial F_B}{\partial \tau} = 0}$$

Don't use these – you may not find an actual optima.

$$\text{Yield} \equiv \frac{F_P}{F_{A_0}}$$

$$\text{Yield}_{A \to P} \equiv X_A S_{A \to P}$$

$$\underset{S_{A \to P}}{\text{Selectivity}} = \frac{F_P}{(F_{A_0} - F_A)}$$

(especially important when A is expensive)

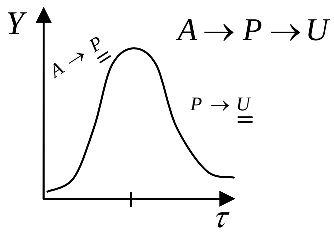

Figure 5. Yield versus residence time. Intermediate P rises in concentration and then falls off as it is converted to U.