

CBE 140 Design Game

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1 Reactor Mass Balance Calculations

1.1 Species Balance on Reactant, A

$$\begin{aligned}a &= i - o + g - c \\0 &= q_{in}C_{0A} - q_{out}C_A - kC_A V \\0 &= qC_{0A} - qC_A - kC_A V \\C_A &= \frac{qC_{0A}}{q + kV} \\C_A &= \frac{C_{0A}}{1 + k\frac{V}{q}}\end{aligned}$$

1.2 Species Balance on Product, D

$$\begin{aligned}a &= i - o + g - c \\0 &= -q_{out}C_D + kC_A V \\0 &= -qC_D + kV \frac{C_{0A}}{1 + k\frac{V}{q}} \\0 &= -qC_D + \frac{C_{0A}}{\frac{1}{kV} + \frac{1}{q}} \\V &= \frac{q}{k} \left(\frac{C_D}{C_{0A} - C_D} \right)\end{aligned}$$

2 Cost Analysis

2.1 Determining the Optimal Conversion Ratio

$$\begin{aligned}
Cost &= q(\Delta t)C_{0A}(Price_A) + V(Cost_{per\ V}) \\
Cost &= q(\Delta t)C_{0A}(Price_A) + \frac{q}{k} \left(\frac{C_D}{C_{0A} - C_D} \right) (Cost_{per\ V}) \\
\frac{Cost}{qC_D} &= \frac{C_{0A}(\Delta t)}{C_D}(Price_A) + \frac{1}{k} \left(\frac{1}{C_{0A} - C_D} \right) (Cost_{per\ V}) \\
\frac{Cost}{qC_D} &= \frac{\Delta t}{X}(Price_A) + \frac{1}{kC_{0A}(1 - X)}(Cost_{per\ V}) \\
\frac{d}{dX} \left[\frac{Cost}{qC_D} \right] &= -\frac{\Delta t}{X^2}(Price_A) + \frac{1}{kC_{0A}(1 - X)^2}(Cost_{per\ V}) \\
0 &= -\frac{\Delta t}{X^2}(Price_A) + \frac{1}{kC_{0A}(1 - X)^2}(Cost_{per\ V}) \\
X &= \sqrt{\frac{(\Delta t)(Price_A)}{\frac{(Cost_{per\ V})}{kC_{0A}} + (\Delta t)(Price_A)}}
\end{aligned}$$

Plugging in $\Delta t = 5.04 \times 10^5 \text{ min}$, $Price_A = \$0.28 \text{ mol}^{-1}$, $Cost_{per\ V} = \$47 \text{ L}^{-1}$, $k = 0.005 \text{ min}^{-1}$, $C_{0A} = 0.20 \text{ mol L}^{-1}$:

$$X = 0.866$$

3 Reactor Sizing (Work in progress)

We will size the reactor to achieve the optimal (cost minimized) conversion ratio, X, when 10% of the time-averaged projected market demand is reached.

$$\begin{aligned}
\bar{D} &= \frac{\Sigma[D_1 \dots D_5]}{5} \\
\bar{D} &= 3.12 \times 10^7 \text{ mol yr}^{-1}
\end{aligned}$$

This amounts to a production rate, qC_D , of:

$$\begin{aligned}
qC_D &= \frac{(0.1)\bar{D}}{(\Delta t)} \\
qC_D &= 6.19 \text{ mol/ min}
\end{aligned}$$

$$V = \frac{1}{k} \frac{qC_D}{C_{0A} - XC_{0A}}$$

$$V = \frac{qC_D}{kC_{0A}(1 - X)}$$

Plugging in $k = 0.005 \text{ min}^{-1}$, $C_{0A} = 0.20 \text{ mol L}^{-1}$, $qC_D = 6.19 \text{ mol/min}$, $X = 0.866$:

$$V = 4.62 \times 10^4 \text{ L}$$