# CBE 140 Design Game

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## 1 Reactor Mass Balance Calculations

### 1.1 Species Balance on Reactant, A

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

### 1.2 Species Balance on Product, D

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

# 2 Cost Analysis

## 2.1 Determining the Optimal Conversion Ratio

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

$Plugging\ in\ \Delta t = 5.04\times10^5\,\mathrm{min},\quad Price_A = \$0.28\,\mathrm{mol^{-1}},\ Cost_{per\ V} = \$47\,\mathrm{L^{-1}},$
$k = 0.005\,\mathrm{min^{-1}},\ C_{0A} = 0.20\,\mathrm{mol\,L^{-1}}:$

$$
\begin{aligned}
\alpha &= -\$1.411\times10^5\,\mathrm{min\,mol^{-1}} \quad \beta = \$4.70\times10^4\,\mathrm{min\,mol^{-1}} \\
X &= \frac{2\alpha \pm \sqrt{(2\alpha)^2 - 4(\alpha+\beta)(\alpha)}}{2(\alpha+\beta)} \\
X &= 0.634
\end{aligned}
$$

# 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.

$$
\begin{aligned}
\bar{D} &= \frac{\Sigma[D_1 \ldots D_5]}{5} \\
\bar{D} &= 3.12\times10^7\,\mathrm{mol\,yr^{-1}}
\end{aligned}
$$

This amounts to a production rate, $qC_D$, of:

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

$$V = \frac{1}{k}\frac{qC_D}{C_{0A} - XC_{0A}}$$
$$V = \frac{qC_D}{kC_{0A}(1 - X)}$$
$$Plugging\ in\ k = 0.005\,\mathrm{min}^{-1},\ \ C_{0A} = 0.20\,\mathrm{mol\,L}^{-1},\ \ \ qC_D = 6.19\,\mathrm{mol/\,min},\ \ \ X = 0.634:$$

$$V = 1.69 \times 10^4\,\mathrm{L}$$

# 4 Year 1 Deliverables

## 4.1 Reactor Volume

$V = 1.69 \times 10^4\,\mathrm{L}$

## 4.2 Product Concentration

$$C_D = C_{0A}X$$
$$C_D = 0.127\,\mathrm{mol\,L}^{-1}$$

## 4.3 Reactor Flow Rate

$$q = \frac{qC_D}{C_D}$$