# Introduction to Reactor Design, 3K4
# Tutorial 3

**Kevin Dunn, kevin.dunn@mcmaster.ca** **Selected questions will be due for assignment 2**

---

**Assignment objectives**: To demonstrate that you understand material on design reactors, and know what rate laws and stoichiometric tables are used for.

### Question 1 [4]

The rote law for the reaction $2\text{A} + \text{B} \longrightarrow \text{C}$ is $-r_A = k_A C_A^2 C_B$ where $k_A = 14\,\text{L}^3.\text{mol}^{-2}.\text{s}^{-1}$.

1. Write the write expression for $-r_B$.
2. And for $+r_C$.
3. What is $k_B$?
4. And $k_C$?

### Question 2 [5]

For the elementary liquid-phase reaction, $A + B \rightleftharpoons C$ with $C_{A0} = C_{B0} = 2\,\text{mol.L}^{-1}$ and $K_C = 10\,\text{L.mol}^{-1}$

1. What is the equilibrium concentrations of all the species?
2. Does it matter in which reactor this occurs? Explain your answer.
3. What is the equilibrium conversion of A?

### Question 3 [10]

Set up a stoichiometric table for the isothermal, isobaric gas-phase pyrolysis of ethane, and express the concentration of each species in the reaction as a function of conversion.

1. Set up the table for a *flow reactor* at 6 atm and 1110K for the reaction: $C_2H_6 \longrightarrow C_2H_4 + H_2$
2. How would your equation for the concentration and reaction rate change if the reaction were to be carried out in a constant-volume batch reactor?

### Question 4 [10]

In the previous tutorial you used the following rate data for $-r_A$ measured in units of $\left[\dfrac{\text{kmol}}{\text{hr.m}^3}\right]$, observed at a particular conversion, $X$:

| Reaction rate | Conversion |
|---|---|
| 78 | 0.0 |
| 106 | 0.2 |
| 120 | 0.4 |
| 70 | 0.6 |

What is the time required for the reaction to reach a 60% conversion of A in a constant volume batch reactor of $2\,\text{m}^2$.

### Question 5 [10]

For the system considered in class previously (see last page of this tutorial's PDF) we have designed a single CSTR to achieve a conversion of 80%. I will teaching in you the 4N4 course how to estimate the capital cost of the CSTR vessel. For now, please use this formula to estimate the capital cost in dollars, in 2011 prices:

$$\text{Cost} = 2800 \cdot \left(\frac{V}{100}\right)^{0.53} \cdot 4 \cdot \left(\frac{1490}{300}\right)$$

where $V$ is the CSTR tank volume, in US gallons (these reason for the formula structure will become clear in the 4N4 course).

1. Estimate the price of a single CSTR to obtain 80% conversion.
2. Estimate the price of two equally-sized CSTR's to obtain 80% conversion. Also write down the reaction rate in the tank, and the conversion leaving each tank.
3. Would it be more economically viable to purchase 3 equally-sizes CSTR's, ordered in series, than to buy a single large CSTR? Show your calculations and explain.

**Table 2-2. Processed Data**

| $X$ | 0.0 | 0.1 | 0.2 | 0.4 | 0.6 | 0.7 | 0.8 |
|---|---|---|---|---|---|---|---|
| $-r_A\left(\frac{\text{mol}}{\text{m}^3\cdot\text{s}}\right)$ | 0.45 | 0.37 | 0.30 | 0.195 | 0.113 | 0.079 | 0.05 |
| $(1/-r_A)\left(\frac{\text{m}^3\cdot\text{s}}{\text{mol}}\right)$ | 2.22 | 2.70 | 3.33 | 5.13 | 8.85 | 12.7 | 20 |
| $(F_{A0}/-r_A)(\text{m}^3)$ | 0.89 | 1.08 | 1.33 | 2.05 | 3.54 | 5.06 | 8.0 |