Lecture 3 (4^{th} of August)

⇨ **Section 3 of the lecture notes – Reaction Rate**

Multiple Reactions

- There are two types of multiple reactions
    - Series
    - Parallel
- There are also combination reactions which combine series and parallel reactions at once.

Series Reactions

- Also called consecutive reactions

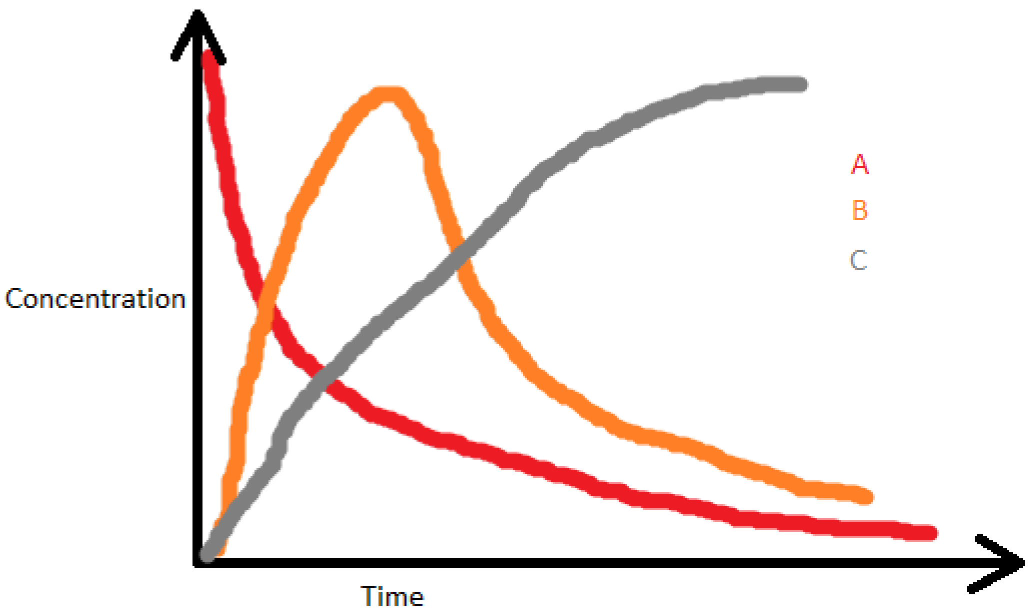
$$A \xrightarrow{k_1} B \xrightarrow{k_2} C$$

For this reaction, the rate equations are given by:

$$r_A = -k_1 C_A$$
$$r_B = k_1 C_A - k_2 C_B$$
$$r_C = k_2 C_B$$

- For series reactions, the most important variable is time. Control the length of time that the reactor is operating and you can control the quantity

A typical graph of the concentrations over time looks like this:



Reactions in Parallel

- An example of these reactions can be:

$$A \xrightarrow{k_B} B \quad \text{desired}$$
$$A \xrightarrow{k_C} C \quad \text{undesired}$$

For this reaction set, the rate laws are given by:

$$r_B = k_B C_A^{\alpha_1}$$
$$r_C = k_C C_A^{\alpha_2}$$

The rate of disappearing A is equivelant to the sum of appearance of C and B:

$$-r_A = r_B + r_C$$
$$= k_B C_A^{\alpha_1} + k_C C_A^{\alpha_2}$$

Where α_1 and α_2 are positive constants

- These reactions are difficult to characterise over time, and as such time is not what is used to control these mechanisms.
  - Use selectivity instead.

Selectivity Parameter:

$$S = selectivity\ parameter = \frac{r_B}{r_C}$$
$$= \frac{k_B}{k_C} C_A^{\alpha_1 - \alpha_2}$$

Of these parameters, C_A is the only quantity that can be adjusted and controlled. The remaining ones are all specific to the system and are temperature dependent.

- If $\alpha_1 > \alpha_2$ and **B** is the desire product (i.e. order of desired is > order of undesired),
  - $\alpha_1 - \alpha_2 = \alpha$ ($\alpha > 0$)
  - Results in:

$$S = \frac{k_B}{k_C} C_A^{\alpha}$$

  - Keep concentration of A as high as possible during reaction
- If $\alpha_1 < \alpha_2$ and B is the desired product
  - $\alpha_1 - \alpha_2 = \alpha$ where $\alpha < 0$

$$S = \frac{k_B}{k_C} * \frac{1}{C_A^{\alpha}}$$

  - Keep A as low as possible (dilute feed with inerts)
- It was mentioned that the other factors (k particularly) were temperature dependent
  - Know this from the Arrhenious Equation

$$\frac{k_B}{k_C} = \frac{A_B}{A_C} * \exp\left(-\frac{E_B - E_C}{RT}\right)$$

  - So if $E_B > E_C$, k_B will increase more rapidly than with increasing temperature so to maximise B, you would run at an elevated temperature.
  - Conversely, if $E_B < E_C$, k_C will increase most rapidly with increased temperature so if B is desired, the rxn should be run at low temperature.