

## Chemical Reaction Engineering

### The rate of a reaction $r_A$

Since chemical reaction engineering concerns itself with the kinetics of the reaction, we must first define what is meant by the "rate of a reaction".

We define the rate of a reaction for component A as follows: "the amount of moles of A disappearing or being generated per unit time per unit volume is the rate of the reaction, denoted as  $r_A$ ".

### Equation for Rate

The rate of a reaction is determined by the rate law. For example, for the reaction,



The rate law could look like,

$$-r_A = k[A]$$

Here,  $[A]$  means the concentration of A in mol/L. We will use  $C_A$  to denote the concentration from now on. So,

$$-r_A = kC_A$$

In this case we say that the reaction is **first order in A**, as the exponent of  $C_A$  is 1. The rate law could also look like,

$$-r_A = kC_A^2$$

In this case, the reaction would be second order in A.

The rate law could also look something like this,

$$-r_A = \frac{k_1 C_A}{1 + k_2 C_A}$$

In which case the order would be hard to determine.

### Rate for components of a reaction

Given the reaction,



The rate laws for each component are related as,

$$\frac{1}{a} r_A = \frac{1}{b} r_B = \frac{1}{c} r_C = \frac{1}{d} r_D$$

### General Mole Balance for a System / Reactor

We now consider a system volume with a species j as shown below:



Figure 1-5 : Mole balance on species j in a system volume, V

The mole balance on this system is,

$$\begin{aligned} & \text{[moles of j in per unit time]} - \text{[moles of j out per unit time]} + \text{[moles of j generated per unit time]} \\ & = \text{[moles of j accumulated per unit time]} \end{aligned}$$

$$F_{j0} - F_j + G_j = \frac{dN_j}{dt}$$

If all the properties of a system, such as catalysis concentration, temperature, concentration of species are uniform throughout the volume, then we can write the  $G_j$  terms simply as the product of  $r_j$  and the system volume V.

$$F_{j0} - F_j + r_j V = \frac{dN_j}{dt}$$

# Chemical Reaction Engineering Notes

**Zhe Xu**



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