Al-Mustaqbal University College
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Chemical Reaction Kinetics

3rd Stage

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Lecture 2

Speed of Chemical Reactions Some reactions occur very rapidly; others very, very slowly. For example, in the production of polyethylene, one of our most important plastics, or in the production of gasoline from crude petroleum, we want the reaction step to be complete in less than one second, while in waste water treatment, reaction may take days and days to do the job. Figure 1.3 indicates the relative rates at which reactions occur. To give you an appreciation of the relative rates or relative values between what goes on insewage treatment plants and in rocket engines, this is equivalent to 1 sec to 3 yr With such a large ratio, of course the design of reactors will be quite different in these cases.

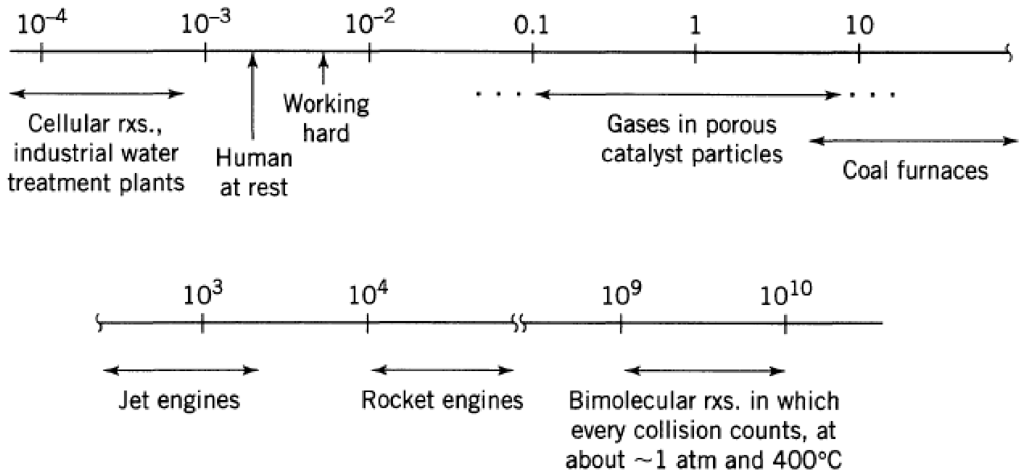

Figure 1.3 Rate of reactions $-r_A''' = \frac{\text{moles of A disappearing}}{\text{m}^3 \text{ of thing} \cdot \text{s}}$

Kinetics of Homogeneous Reactions

The Rate Equation

Suppose a single-phase reaction

$$aA + bB \rightarrow rR + sS.$$

The most useful measure of reaction rate for reactant A is then;

$$-r_A = -\frac{1}{V}\frac{dN_A}{dt} = \frac{\text{(amount of A disappearing)}}{\text{(volume) (time)}}, \quad \left[\frac{\text{mol}}{\text{m}^3 \cdot \text{s}}\right] \qquad \textbf{(1)}$$

rate of disappearance of A

note that this is an intensive measure

the minus sign means disappearance

In addition, the rates of reaction of all materials are related by

$$\frac{-r_A}{a} = \frac{-r_B}{b} = \frac{r_R}{r} = \frac{r_S}{s}$$

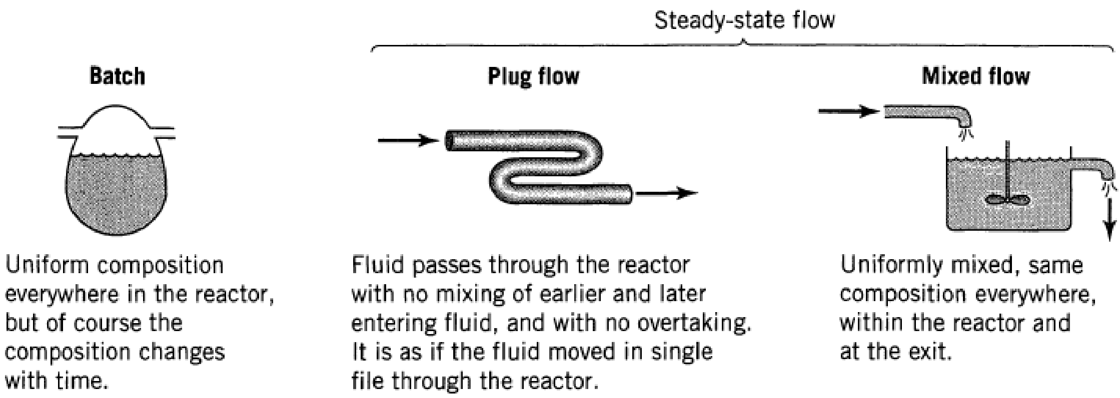

Figure 2.1 Ideal reactor types.

Experience shows that the rate of reaction is influenced by the *composition* and the *energy of the material.* By energy we mean the temperature (random kinetic energy of the molecules), the light intensity within the system (this may affect the bond energy between atoms), the magnetic field intensity, etc. Ordinarily we only need to consider the temperature, so let us focus on this factor. Thus,
we can write;

$$\frac{mol}{m^3 \cdot s} \quad -r_A = f\begin{bmatrix} \text{temperature dependent terms}, & \text{concentration dependent terms} \end{bmatrix} \xlongequal[\text{example}]{\text{as an}} kC_A^a = k_0 e^{-E/RT} C_A^a \qquad \textbf{(2)}$$

$\left(\frac{mol}{m^3}\right)^{1-a} s^{-1}$

activation energy

reaction order

temperature dependent term

Conversion , and yield

Conversion, X, is defined as the fraction (or percentage) of the more important or limiting reactant that is consumed. With two reactants A and B and a nearly Stoichiometric feed, conversions based on each reactant could be calculated.

$$X = \frac{\text{mole A reacted}}{\text{mole A fed}} \qquad \text{….3}$$

Yield, Y, is the amount of desired product produced relative to the amount that would have been formed if there were no byproducts and the main reaction went to completion

$$Y = \frac{\text{moles of product formed}}{\text{maximum moles of product, x = 1.0}} \qquad \text{…4}$$

Conceptes of Kinetics

1. Stoichiometry.

Consider the general reaction;

$$aA + bB \rightarrow cC + dD$$

on a “per mole of A basis”…i.e assume A is the limiting reactant :-

$$A + \left(\frac{b}{a}\right)B \rightarrow \left(\frac{c}{a}\right)C + \left(\frac{d}{a}\right)D$$

where the Stoichiometric Coefficients ,

$$\left(\frac{b}{a}\right), \left(\frac{c}{a}\right), \left(\frac{d}{a}\right)$$

Molecules are lost and formed by reaction , and mass conservation requires that amounts of species are related by Stoichiometry as:-

1 mole of A and $\left(\frac{b}{a}\right)$ of B consumed , while $\left(\frac{c}{a}\right)$mole of C and $\left(\frac{d}{a}\right)$ mole of D formed or appear

Rate of reaction or disappearance of A $= -r_A \ \frac{mole}{m^3.time}$

Rate of formation of C$(r_C) = \left(\frac{c}{a}\right)(-r_A) \ \frac{mole}{m^3.time}$

Rate of formation of D$(r_D) = \left(\frac{d}{a}\right)(-r_A) \ \frac{mole}{m^3.time}$

Also, Rate of formation of C $(r_C) = \left(\frac{c}{d}\right)(r_D)$

Rate of formation of D $(r_D) = \left(\frac{d}{c}\right)(r_C)$

Then the reaction Stoichiometry; $\frac{-r_A}{a} = \frac{-r_B}{b} = \frac{r_C}{c} = \frac{r_D}{d}$

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

EXAMPLE

When butane is burned it decreases at a rate of 0.20 mol/s.

$$2\ C_4H_{10}\ (g) + 13\ O_2\ (g) \rightarrow 8\ CO_2\ (g) + 10\ H_2O\ (g)$$

(butane)

a. What is the rate at which O_2concentration is decreasing?
b. What are the rates at which the product concentrations are increasing?

Answers:
a. 0.20 M/s * 13/2 = 1.3 M/s is the rate that $O_2$is consumed.
b. 0.20 M/s * 8/2 = 0.8 M/s is the rate that $CO_2$is produced.
0.20 M/s * 10/2 = 1.0 M/s is the rate that H_2O is produced.