Chapter 2: Reaction Kinetics

Reaction kinetics is the study of the speed at which reactions occur or proceed. The rate of a reaction is used to denote the formation or disappearance (removal) of a compound.

Homogenous reactions – reactions that take place in a single phase (liquid, gas or solid)

Heterogeneous Reactions - reactions that occur at surfaces between phases

Production is denoted as +

Removal is denoted as –

Reaction Rates are a function of temperature, pressure and concentration of reactants.

A general mathematical expression describing the reaction rate (r) at which the mass or volume of a material A is changing with time is given as

$$dA/dt = r$$

When r= k, a constant the reaction is a Zero Order Reaction

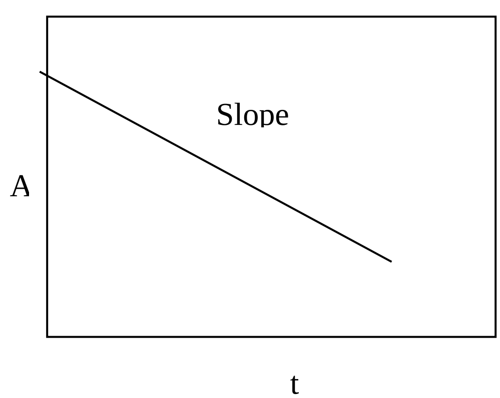
If the concentration of A at time 0 is Ao and and time t is At and A is being removed, the integrated form of the zero order reaction is

$$\int_{Ao}^{At} dA = \int_{0}^{t} -k\,dt$$

or $A_t - A_o = -kt$

or $A_t = A_o - kt$

This is a equation of a straight line and can be plotted as follows:



First order reactions are reactions where the rate of change of A is proportional to the quantity of component A

Thus $dA/dt = -kA$ represents a First order reaction

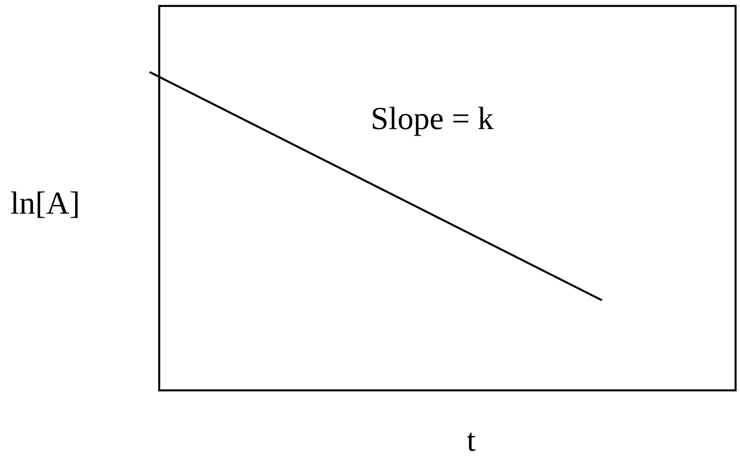
Rearranging and integrating again yields

$$\int_{Ao}^{At} \frac{dA}{A} = \int_{0}^{t} -k\,dt$$

$\ln A - \ln A_0 = -kt$

or $\ln A = \ln A_0 - kt$

Similarly a plot of lnA versus time will yield



Like the zero and first order reactions, $dA/dt = kA^2$ represents a Second order reaction

Things to remember

Units of k for a zero order reaction is concentration/time

Units of k for a first order reaction is 1/time

Example Problems:

1) In a first order process a blue dye reacts to form a purple dye. The amount of blue at the end of an hour is 480 g and at the end of 3 hours is 120 g. Estimate the initial amount of dye and the reaction rate.

Let initial dye concentration be Ao

Therefore $\ln(480) = \ln(Ao) - k(1)$ [1]

Similarly, $\ln(120) = \ln(Ao) - k(3)$ [2]

Solving the two equations we get $k = 0.693\ min^{-1}$ $Ao = 959$ mg/L

2) **Data for removing "Gobbledygook" was obtained and is shown below. Determine the reaction order and the reaction rate.**

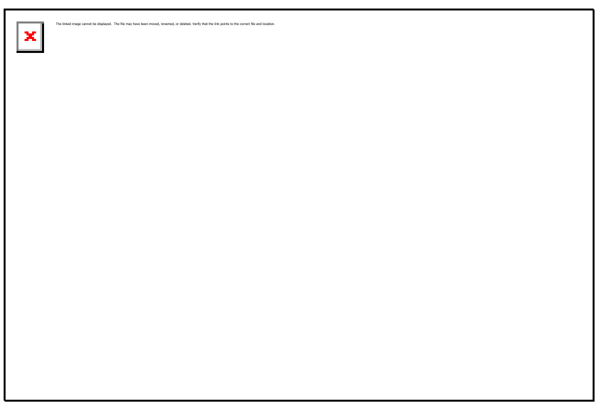
Time min	Gobbledygook mg/L
0	170
5	160
10	98
20	62
30	40
40	27

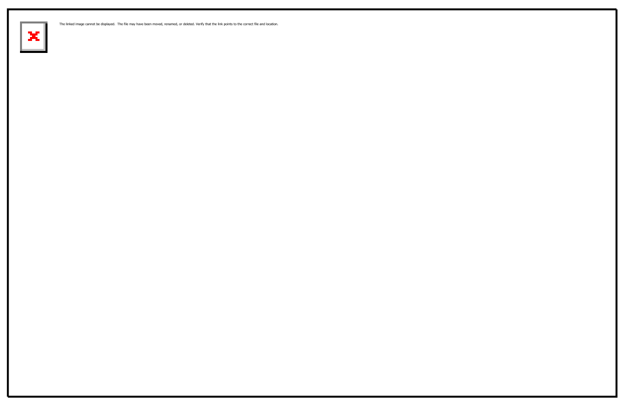
Solution:

Calculate ln (Gook)

Plot G vs T and Ln G vs t to determine reaction order.

Time min	Gook mg/L	Ln(Gook)
0	170	5.135798
5	160	5.075174
10	98	4.584967
20	62	4.127134
30	40	3.688879
40	27	3.295837





Better correlation when plotted ln (g) vs. time. Therefore reaction is first order.

Reaction rate is slope of line = 0.0481 1/minute