Chemistry 146 Lecture Problems
Integrated Rate Equation

Integrated Rate Equation: For a first order reaction with rate constant (k). After time (t) the initial concentration (A_0) will change to the new concentration at time t (A_t).

The rate of formation of X from the chemical reaction: A --> X where the initial concentration of A is A_o and the initial concentration of X is 0. The concentration of X at time t is X(t). The concentration of A at time t is A(t)

The rate of a reaction is:

$$rate = \frac{\Delta X}{\Delta t}$$

The rate for a first order reaction is:

$$rate = k \cdot A(t)$$

These two may be combined as:

$$\frac{\Delta X}{\Delta t} = k \cdot A(t)$$

The concentration of A at time t may also be written in terms of X (the amount that has reacted) since the area under a plot of [A] vs time is the amount that has reacted. Then this may be integrated as:

$$A(t) = A_o - X(t)$$

So the above equation may be rewritten as:

$$\frac{\Delta X}{\Delta t} = k\left(A_0 - X(t)\right)$$

Which rearanges to:

$$\frac{1}{A_0 - X(t)} \cdot \Delta X = k \cdot \Delta t$$

In calculus an extremely small change in x (little Δx) is written as dx. Rewriting the above in this notation for a very small change in x and t (If you have not taken calculus just bear with us here, I will try and explain it another way shortly) and then integrate the function:

$$\int \frac{1}{A_0 - X} dX = \int k\,dt$$

$$-\ln\left(A_0 - X\right) = k \cdot t$$

Don't forget the integration constant which would give:

$$-\ln\left(A_0 - X\right) = k \cdot t + C$$

The integration constant may be evaluated knowing that at t=0, x=0 so that

$$-\ln(A_0 - 0) = k\cdot 0 + C$$

$$C = -\ln(A_0)$$

Substitute this expression into the above so that:

$$-\ln(A_0 - X) = k\cdot t + -\ln(A_0)$$

This rearanges to give:

$$\ln(A_0) - \ln(A_0 - X) = k\cdot t$$

$$\ln\left(\frac{A_0}{A_0 - X}\right) = k\cdot t$$

Since A_o-X at time t is also A(t), this may be rewritten as follows:

$$\ln\left(\frac{A_0}{A(t)}\right) = k\cdot t$$ this is the integrated rate equation:

Which rearanges as follows for different applications:

$$t = \ln\left(\frac{A_0}{A(t)}\right)\cdot\frac{1}{k} \qquad a_0 = e^{k\cdot t}\cdot A(t) \qquad A(t) = a_o\cdot e^{-k\cdot t}$$

For a sample problem with the integrated rate equation. For the reaction:
$C_2H_5Cl \rightarrow C_2H_4 + HCl$ at 700 K, k = $2.50*10^{-3}$ min^{-1}

If the initial concentration of C_2H_5Cl is 3.45 atm, how long does it take for the partial pressure of C_2H_5Cl to drop to 1.00 atm?

Given in the problem:

$A_0 := 3.45\cdot atm$

$A_t := 1.00\cdot atm$

$k := 2.50\cdot 10^{-3}\cdot min^{-1}$

The integrated rate equation (rearanged to solve for time)

$$t := \ln\left(\frac{A_0}{A_t}\right)\cdot\frac{1}{k}$$

$t = 495.34969\cdot min$

What is the partial pressure of C_2H_5Cl after six hours?

$t := 6 \cdot hr$ $t = 360 \cdot min$

$A_t := A_0 \cdot e^{-k \cdot t}$

$A_t = 1.40267 \cdot atm$

How long does it take for the C_2H_5Cl concentration to drop to 1/2 the initial concentration?

$A_t := \frac{1}{2} \cdot A_0$

$t := \ln\left(\frac{A_0}{A_t}\right) \cdot \frac{1}{k}$

$t = 277.25887 \cdot min$

How long does it take for 99% of the C_2H_5Cl to react?

$A_t := 1 \cdot \% \cdot A_0$

$t := \ln\left(\frac{A_0}{A_t}\right) \cdot \frac{1}{k}$

$t = 1.84207 \cdot 10^3 \cdot min$

Now an example of how the integrated rate equation is used to calculate the concentration of a at time t

$$A_0 := 0.0100 \cdot \text{mole} \cdot \text{liter}^{-1}$$

$$k := 2.50 \cdot 10^{-3} \cdot \text{min}^{-1}$$

$$A(t) := A_0 \cdot e^{-k \cdot t}$$

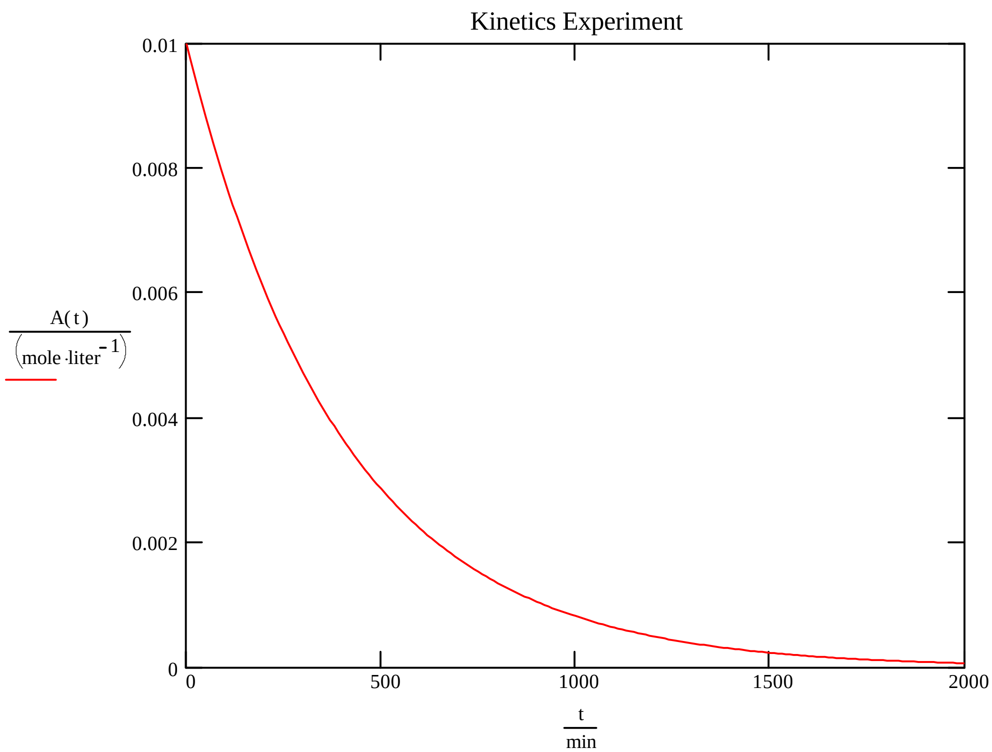
$$A(0 \cdot \text{min}) = 0.01 \cdot \text{mole} \cdot \text{liter}^{-1}$$

$$A(1 \cdot \text{min}) = 9.97503 \cdot 10^{-3} \cdot \text{mole} \cdot \text{liter}^{-1}$$

$$A(10 \cdot \text{min}) = 9.7531 \cdot 10^{-3} \cdot \text{mole} \cdot \text{liter}^{-1}$$

$$A(100 \cdot \text{min}) = 7.78801 \cdot 10^{-3} \cdot \text{mole} \cdot \text{liter}^{-1}$$

$$t := 0 \cdot \text{min}, 10 \cdot \text{min} .. 2000 \cdot \text{min}$$



Using similar equations the concentration of the product x is:

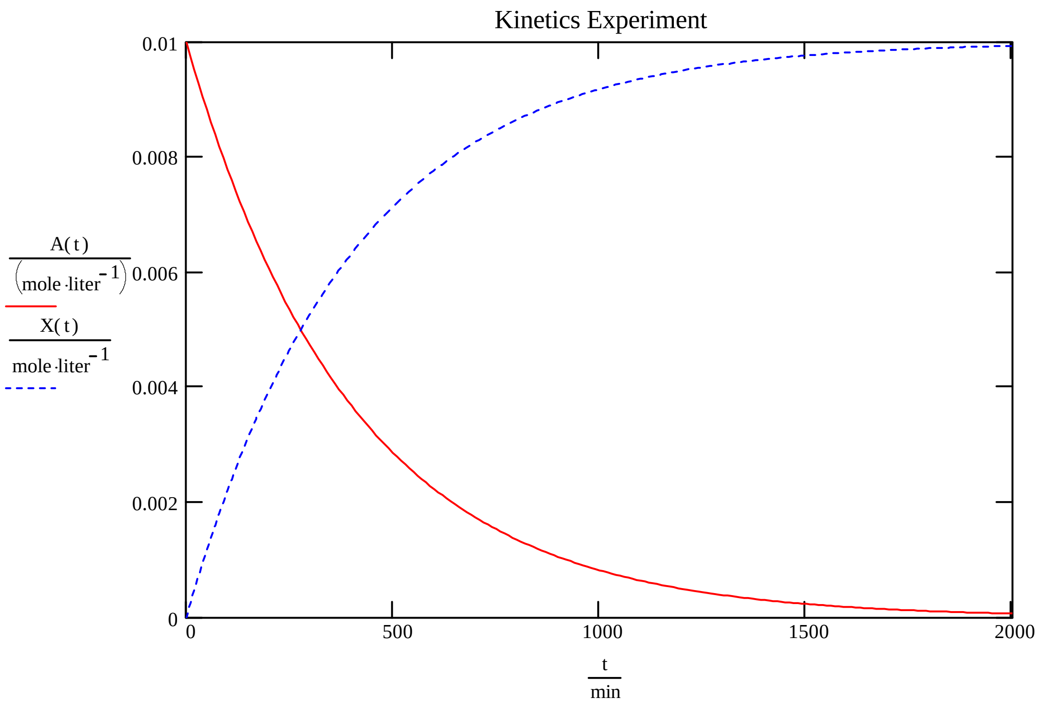
$$X(t) := A_0 - A_0 \cdot e^{-k \cdot t}$$

$X(0 \cdot min) = 0 \cdot mole \cdot liter^{-1}$

$X(1 \cdot min) = 2.49688 \cdot 10^{-5} \cdot mole \cdot liter^{-1}$

$X(10 \cdot min) = 2.46901 \cdot 10^{-4} \cdot mole \cdot liter^{-1}$

$X(100 \cdot min) = 2.21199 \cdot 10^{-3} \cdot mole \cdot liter^{-1}$



The integrated rate equation may also be used as follows:

The time required for the concentration of A to drop to one half the initial concentraiton:

$$A(t) = \frac{1}{2} \cdot A(0)$$

$$t = \ln\left(\frac{A(0)}{A(t)}\right) \cdot k^{-1}$$

$$t = \ln\left(\frac{1}{0.5}\right) \cdot k^{-1}$$

$$t = \ln(2) \cdot k^{-1}$$

$$t = \frac{.6931471806}{k}$$

For $k := 1 \cdot sec^{-1}$

$$t := \frac{.6931471806}{k}$$

$$t = 0.69315\ sec$$

The time required for the concentration of A to drop to one tenth the initial concentraiton:

$$A(t) = \frac{1}{10} \cdot A(0)$$

$$t = \ln\left(\frac{A(0)}{A(t)}\right) \cdot k^{-1}$$

$$t = \ln\left(\frac{1}{0.1}\right) \cdot k^{-1}$$

$$t = \ln(10) \cdot k^{-1}$$

$$t = \frac{2.302585093}{k}$$

For $k := 1 \cdot sec^{-1}$

$$t := \frac{2.302585093}{k}$$

$$t = 2.30259\ sec$$