What is the reaction rate model for this reversible elementary reaction?

2A + B <-> C

Rate Equation

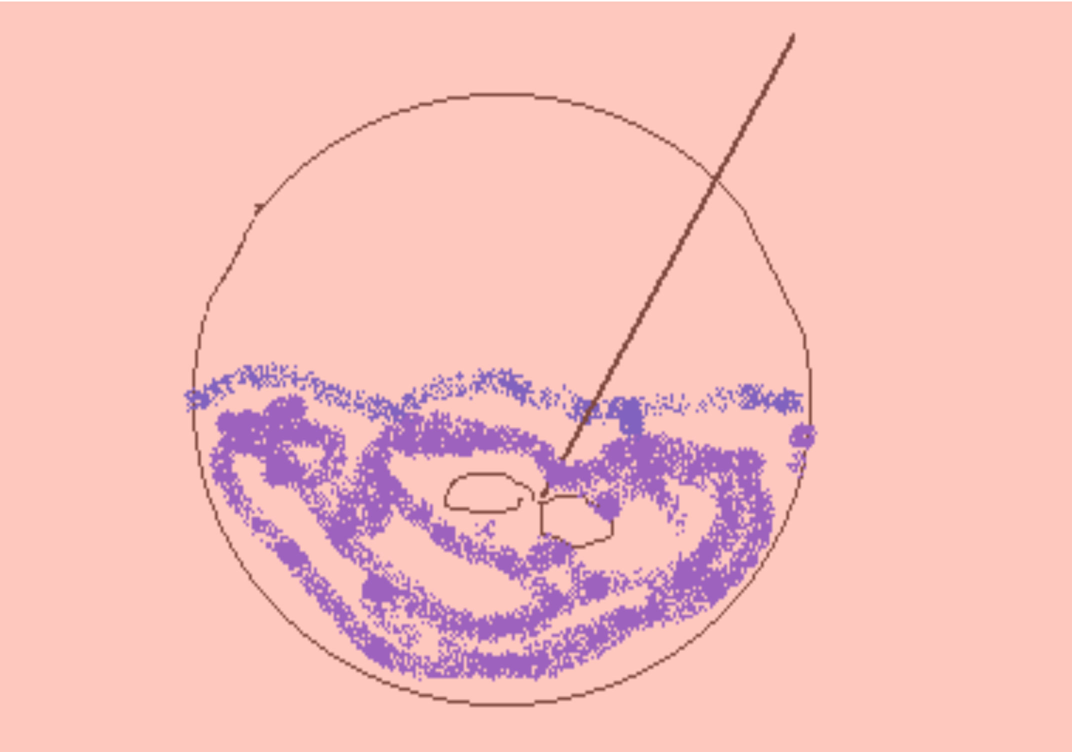
- The determination of the rate equation follows a two-step procedure
  - the concentration dependency is found at fixed temperature
  - the temperature dependence of the rate constants is found

$$\begin{aligned} r_i &= f_1(\text{temperature}) \cdot f_2(\text{composition}) \\ &= k \cdot f_2(\text{composition}) \end{aligned} \tag{33}$$

Batch Reactor

Ideal batch reactor

Assumptions:
Composition varies with time
Uniform composition
Constant volume
Usually operated isothermally



- **Very simple**
- **Need very little supporting equipment**
- **Ideal for small-scale experimental studies on rxn kinetics**

Constant-Volume Batch Reactor

When we mention the constant-volume batch reactor we are really referring to the volume of reaction mixture, and not the volume of reactor. Thus, this term actually means a *constant-density reaction system*. Most liquid-phase reactions as well as all gas-phase reactions occurring in a constant-volume bomb fall in this class.

In a constant-volume system the measure of reaction rate of component i becomes

$$\boxed{r_i = \frac{1}{V}\frac{dN_i}{dt} = \frac{d(N_i/V)}{dt} = \frac{dC_i}{dt}} \qquad \textbf{(1)}$$

Conversion

Suppose that N_{A0} is the initial amount of A in the reactor at time $t = 0$, and that N_A is the amount present at time t. Then the conversion of A in the constant volume system is given by

$$X_A = \frac{N_{A0} - N_A}{N_{A0}} = 1 - \frac{N_A/V}{N_{A0}/V} = 1 - \frac{C_A}{C_{A0}} \tag{7}$$

and

$$dX_A = -\frac{dC_A}{C_{A0}} \tag{8}$$

Measuring how far a reaction has occurred

Concentration (C) – start at Co, end at C

Conversion (X) – start at 0, goes up to 1

$$X = (Co\text{-}C)/Co = 1 – C/Co$$

Extent of reaction (ξ) – starts at 0, goes up to infinity

$$\xi = (N_i – N_{io})/\nu_i \quad \text{(component i)}$$

First-order Reactions

Irreversible Unimolecular-Type First-Order Reactions. Consider the reaction

$$A \rightarrow \text{products} \tag{9}$$

Suppose we wish to test the first-order rate equation of the following type,

$$-r_A = -\frac{dC_A}{dt} = kC_A \tag{10}$$

Separating and integrating:

$$-\int_{C_{A0}}^{C_A} \frac{dC_A}{C_A} = k \int_0^t dt$$

or

$$-\ln \frac{C_A}{C_{A0}} = kt \qquad \textbf{(11)}$$

In terms of conversion (see Eqs. 7 and 8), the rate equation, Eq. 10, becomes

$$\frac{dX_A}{dt} = k(1 - X_A)$$

which on rearranging and integrating gives

$$\int_0^{X_A} \frac{dX_A}{1 - X_A} = k \int_0^t dt$$

or

$$\boxed{-\ln(1 - X_A) = kt} \tag{12}$$

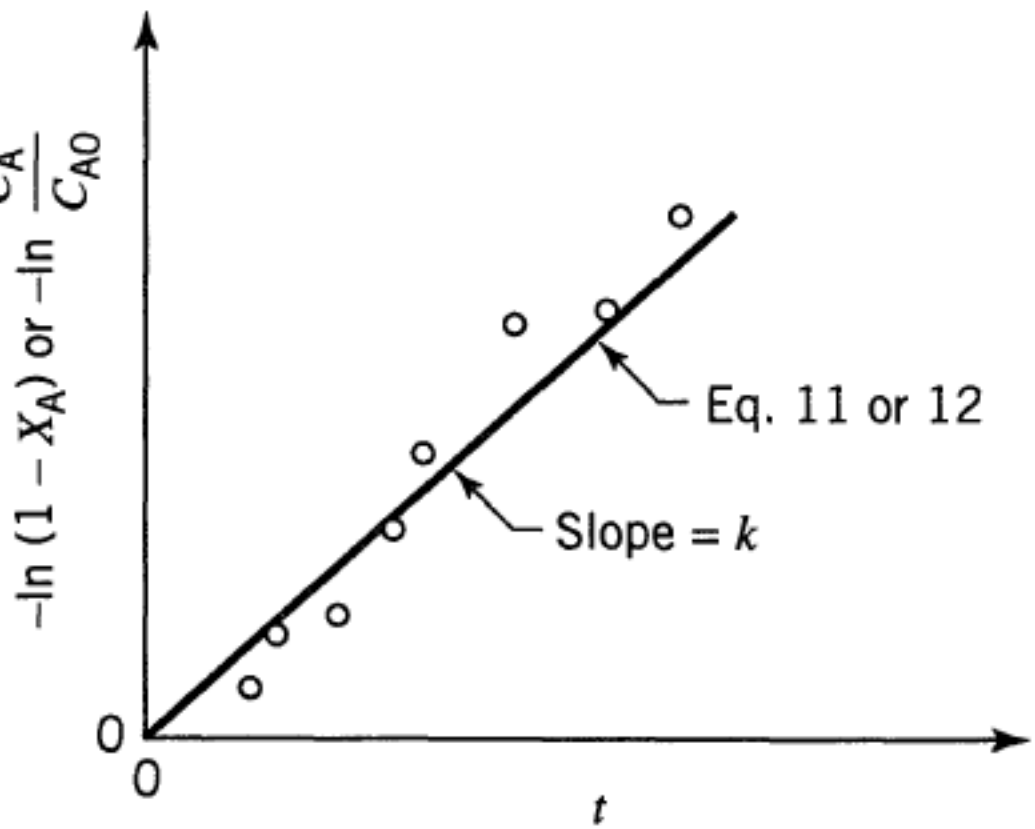


Figure 3.1 Test for the first-order rate equation, Eq. 10.

First order reaction solution

$-r_i = k*C_i$

$-r_i = k*C_{io}*(1\text{-}X)$

$-r_i = k*(C_{io}+\nu_i\xi/V)$ (V = volume of reaction mixture)

$C_{i=}C_{io*}e^{-kt}$

$X = 1\text{-}e^{-kt}$

$\xi\ = VC_{io}/\nu_i*(-1+e^{-kt})$

What about other reaction rate equations?