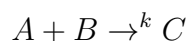


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Chemical Kinetics

Chemical reactions, well-stirred (no diffusion)
 Reactions occur due to collision between the molecules



where k is the rate.

How does the reaction proceed – *to track!* Use concentration of the chemicals

Notation: $A(t)$ = concentration of A

$$[A] = \frac{\text{moles}}{\text{concentration}^3}$$

$$\frac{dA}{dt} = \frac{dB}{dt} = -\frac{dC}{dt} \quad (1)$$

Simple Reactions

0.2.1 1st order: $A \rightarrow^k B$ (radioactive decay)

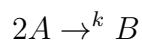
$$\frac{dA}{dt} \propto A$$

$$\frac{dA}{dt} = kA^1$$

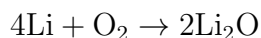
$$A = ce^{-kt}$$

$$\ln A = -kt + c$$

0.2.2 2nd order: $A + A \rightarrow^k B$



$$\frac{dA}{dt} = -2kA^2$$



The stoichiometric coefficients are 4, 1, and 2.

Goal: Track concentrations of chemicals in time (similar to drug care)

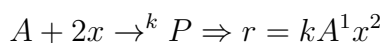
Law of Mass Action

- 1) The rate r of the reaction is proportional to the product of the reactant concentrations, with each concentration raised to the power equal to its respective stoichiometric coefficient.
- 2) The rate of change of the concentration of each species in the reaction is the product of its stoichiometric coefficients with the rate of the reaction adjusted for sign ($-$ for reactant, $+$ for product).
- 3) For a system of reactions,



Using (2):

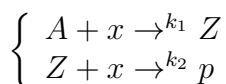
$$\begin{aligned} \frac{dA}{dt} &= -\alpha r \\ &= -\alpha k A^\alpha B^\beta \\ \frac{dB}{dt} &= -\beta k A^\alpha B^\beta \\ \frac{dC}{dt} &= \gamma k A^\alpha B^\beta \\ \frac{dD}{dt} &= \delta k A^\alpha B^\beta \end{aligned}$$



This is highly unlikely given that the reaction would need 2 x 's to come into contact with an A at the same time.

Reaction may proceed in elementary steps!

True mechanism



where z is an intermediate complex! This mechanism only involves binary collisions.

$$\text{Law of mass Action} \Rightarrow \begin{cases} \frac{dA}{dt} = -k_1 Ax \\ \frac{dx}{dt} = -k_1 Ax - k_2 zx \\ \frac{dz}{dt} = k_1 Ax - k_2 zx \\ \frac{dP}{dt} = k_2 zx \end{cases}$$

4 ODE's – nonlinear (hard)

Initial conditions: $A(0) = A_0$, $x(0) = x_0$, $z(0) = 0$, $P(0) = 0$.

How do we expect the concentration to change in time.

How to analyze a nonlinear, system of ODE's.

Strategy: Reduce the number of equations: **compression**.