Chemical Reactions & Differential Equations

\[ A + B \xrightarrow{K_*} C \quad \text{chemical A + chemical B react to produce C.} \]

Mass-action kinetics - reaction rate is proportional to the product of the concentrations of the reactants.

Let \( a = \text{conc. of A} \)
\( b = \text{conc. of B} \)
\( c = \text{conc. of C} \)

\[ \frac{dc}{dt} = K_* \, ab \]

Conservation of mass gives
\[ a + c = a_T \]
\[ \text{total a in system (free + complex)} \]
\[ \text{free a} \quad a \text{ in complex with b} \]

Similarly
\[ b + c = b_T \]

Use conservation to eliminate \( a + b \) to get
\[ \frac{dc}{dt} = K_* (a_T - c)(b_T - c) \]

Can solve this for \( c \), given initial conditions
Reversible reaction

\[ A + B \xrightleftharpoons[k_-]{k_+} C \]

\[
\frac{dC}{dt} = k_+ (a_T - C)(b_T - C) - k_- C
\]

production of C  loss of C from
from forward reaction  backward reaction

Can solve this by separating and integrating

This equilibrium is stable
Note: \( C < \min(a_T, b_T) \) & so reaction will approach this equilibrium.
Enzymatic Reactions

Enzymes are molecules that catalyze (promote) chemical reactions.

\[ X + E \overset{\text{C}}{\rightarrow} P + E \]

\( X + E \) come together to form the intermediate complex \( C \). Then the complex is transformed into the product \( P \) and the enzyme is released.

Not interested in the intermediate complex.

Write \( X \rightarrow P \)

with Michaelis-Menten Kinetics

\[ \frac{dP}{dt} = \frac{KE_x}{K_s + x} = \frac{V_{\text{max}} x}{K_s + x} \]

where \( V_{\text{max}} \) is the maximum reaction rate.

Notice that the reaction rate approaches \( V_{\text{max}} \) as \( x \rightarrow \infty \). Lots of substrate (i.e. \( x \)), but only so much enzyme around to catalyze the reaction.

More \( x \) will not speed this up if few enzymes around.
Cooperativity — sigmoidal kinetics

Suppose enzyme binds multiple molecules of the substrate before catalyzing the reaction.

\[ 2X + 3 \rightleftharpoons C \rightarrow 2P + 3 \]

\[ \cdot \bigcirc \rightarrow \cdot \bigcirc \rightarrow \cdot \bigcirc \cdot \]

\[ X \rightarrow P \] with reaction rate given by

\[ \frac{dP}{dt} = \frac{KeX^2}{(K_s)^2 + X^2} = \frac{V_{max}X^2}{K_s^2 + X^2} \]
Example: Chemical Switch

Suppose a chemical signal leads to the production of chemical $X$ at a rate $K_s$, where $s$ is the strength of the signal. $X$ is autocatalytic and produces more $X$ with sigmoidal kinetics, and it is degraded at a rate proportional to its concentration.

\[
\frac{dx}{dt} = K_s s + \frac{K_2 x^2}{K_b^2 + x^2} - K_3 x
\]

- **Input signal**
- **Positive feedback**
- **Amplifies signal**
- **$x$ produces more $x$**
- **Constant degradation**

Look at equilibrium value of $x$ as a function of the input signal $s$.

Increasing $s$ moves the production up.

Low signal - one stable equilibrium
Equilibria are solutions to

$$k_1 S + \frac{k_2 x^2}{k_5^2 + x^2} - k_3 x = 0$$
Suppose solution is at the low equilibrium and S is in the range where there are three equilibria.

To "turn on" the production of X, S can be increased to "switch" the solution to the high equilibrium. S can decrease and the value of X will stay high, unless S is reduced too much.

Diagram:
- External stimulus
  - Increase S
  - X moves to low equilibrium
- Return to resting S
- Decrease in S
  - X now at high equilibrium
- New equilibrium
  - Decrease S to starting value
  - X now at high equilibrium