Compartment

A dynamic entity such as a level, concentration or number.

Value in compartment is controlled by a differential equation:

\[
\frac{d\text{Compartment}}{dt} = f(t)
\]

Or usually…

\[
\frac{dx}{dt} = \Sigma \text{inflows} - \Sigma \text{outflows}
\]
Compartments: Population Growth

\[ \frac{d\text{Population}_\text{size}}{dt} = \text{Births} - \text{Deaths} \]

- Births = birth_rate \* Population_size
  - birth_rate is a constant based on the biology of individuals
- Deaths = death_rate \* Population_size
  - death_rate is a constant based on the biology of individuals

- Initial size = 1
- birth_rate = 0.3
- death_rate = 0.1
When these balls collide they produce light as a product and die in the process. One white ball (W) colliding with one black ball (B) produces one photon of light (L). The rate at which light is produced by colliding balls is $k$.

Can you draw a graph that would show the rate of light production over time with these initial conditions and no new production of balls.

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**Mass Action**

Law of mass action states that the rate of a reaction is proportional to an integral power of the concentrations of all the substances taking part in the reaction.

E.g., for $A + B \xrightarrow{k_1} C$ the differential equ for $C$ is:

$$\frac{dC}{dt} = k_1 AB - k_{-1} C,$$

where $k_1$ is the constant relating to the rate of production of $C$ when $A$ binds with $B$; and $k_{-1}$ is the constant relating to rate of release of $A$ and $B$ from $C$. 

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Mass Action

E.g., for \( A + 2B \overset{k_1}{\underset{k_{-1}}{\rightleftharpoons}} C \) the differential equ for \( C \) is:

\[
\frac{dC}{dt} = k_1 AB^2 - k_{-1} C,
\]

where \( B \) is raised to the power of 2 because 2 molecules of \( B \) are required.

Enzyme activity or Protein transfer

- Concentration of Substrate (\( S \)),
- Concentration of Enzyme (\( X_0 \)),
- Enzyme bound to substrate (\( X_1 \)),
- Concentration of Product (\( P \)).

\[
S + X_0 \overset{k_1}{\underset{k_{-1}}{\rightleftharpoons}} X_1 \overset{k_2}{\rightarrow} P + X_0
\]
\[
S + X_0 \quad \xrightarrow{k_1} \quad X_1 \quad \xrightarrow{k_2} \quad P + X_0
\]

\[
\begin{align*}
\frac{ds}{dt} &= -k_1 s x_0 + k_{-1} x_1 \\
\frac{dx_1}{dt} &= +k_1 s x_0 - k_{-1} x_1 - k_2 x_1 \\
\frac{dp}{dt} &= +k_2 x_1 
\end{align*}
\]
Enzyme Kinetics

In our previous problem of enzyme and substrate, let us assume two molecules of substrate are required by the enzyme. In this case, our reaction becomes the following with the corresponding differential equation below:

\[
2S + X_0 \xrightarrow{k_1} X_1 \xrightarrow{k_2} 2P + X_0
\]

\[
\frac{dc}{dt} = -k_1S^2x_0 + k_2x_1
\]

\[
\frac{dx_1}{dt} = +k_1S^2x_0 - k_2x_1 - k_2x_1
\]

Protein transfer across a membrane via a receptor

- Concentration of protein (S),
- Concentration of receptors on membrane (X_0),
- Receptor bound to protein (X_1),
- Transfer of protein across membrane (P).

\[
S + X_0 \xrightarrow{k_1} X_1 \xrightarrow{k_2} P + X_0
\]
Saturation Feedback

- E.g., Transfer of a protein across a membrane via a receptor:
- Basic equation Michaelis-Menten equation applies:

\[ V = \frac{V_{max} \cdot S}{K_m + S} \]

- \( V = \) rate of product formation
- \( V_{max} = \) max reaction velocity
- \( S = \) substrate concentration
- \( K_m = \) half saturation constant; low \( K_m \) is a rapidly rising curve