Modeling Biochemical Networks Cheat Sheet[1]

Stoichiometric Amount

The stoichiometric amount is the number of molecules of a particular reactant or product taking part in a reaction.

e.g.

$2A + 4B \longrightarrow 3C$

Stoichiometric amount of $A = 2; B = 4$ and $C = 3$.

Stoichiometric Coefficient

The stoichiometric coefficient, c, of a species X is the difference between the stoichiometric amount of species on the product side minus the stoichiometric amount of the same species on the reactant side.

e.g.

$A \longrightarrow B$

$c_A = 0 - 1 = -1$

$c_B = 1 - 0 = 1$

$2A + B \longrightarrow C$

$c_A = 0 - 2 = -2$

$c_B = 0 - 1 = -1$

$c_C = 1 - 0 = 1$

Reaction Rate

$A \xrightarrow{v} B$

Units: mol per time per volume, defined as:

$$v = \frac{1}{c_X}\frac{dX}{dt}$$

Rate of Change

The rate of change of a substance X is

$$\frac{dX}{dt} = c_X v$$

where c_X is the stoichiometric coefficient for X.

α is usually $\oplus$ for products.

α is usually $\ominus$ for reactants.

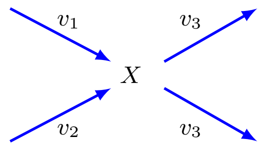
e.g.

$2A \longrightarrow B$

$$\frac{dA}{dt} = -2v \qquad \frac{dB}{dt} = v$$

[1] Version 0.5

Mass Conservation



$$\frac{dX}{dt} = (v_1 + v_2) - (v_3 + v_4)$$

In general:

$$\frac{dX}{dt} = \text{Flows In} - \text{Flows Out}$$

Rate Laws

Mass-action: $v = kA^{m_1}B^{m_2}\ldots$

Mass-action reversible:

$v = k_1A^{m_1}B^{m_2}\ldots - k_2P^{n_1}Q^{n_2}\ldots$

e.g.

$A \longrightarrow B \qquad v = k_1A \quad [-k_2B]$

$2A \longrightarrow B \qquad v = k_1A^2 \quad [-k_2B]$

$2A + B \longrightarrow C \qquad v = k_1A^2B \quad [-k_2C]$

$2A + B \longrightarrow C + D \qquad v = k_1AB \quad [-k_2CD]$

Equilibrium Constant

$$K_{eq} = \frac{P^{n_1}Q^{n_2}\ldots}{A^{m_1}B^{n_2}\ldots}$$

e.g.

$A \longrightarrow B \quad K_{eq} = \dfrac{B}{A}$

$A + B \longrightarrow C \quad K_{eq} = \dfrac{C}{AB}$

$A + A \longrightarrow B \quad K_{eq} = \dfrac{B}{A^2}$

Mass-Action Ratio

For a reaction such as $A \longrightarrow B$, the mass-action ration, Γ is given by:

$$\Gamma = \frac{B}{A}$$

where A and B are at their *in vivo* concentrations.

Dissequilibrium Ratio

$$\rho = \frac{\Gamma}{K_{eq}}$$

At equilibrium, $\rho = 1$, if out of equilibrium then $\rho < 1$.

Rates of Change and Rates Laws

$A \longrightarrow B \quad \dfrac{dA}{dt} = -v \quad \dfrac{dB}{dt} = v$

$A + B \longrightarrow C \quad \dfrac{dA}{dt} = -v \quad \dfrac{dB}{dt} = -v \quad \dfrac{dC}{dt} = v$

$A + A \longrightarrow B \quad \dfrac{dA}{dt} = -2v \quad \dfrac{dB}{dt} = v$

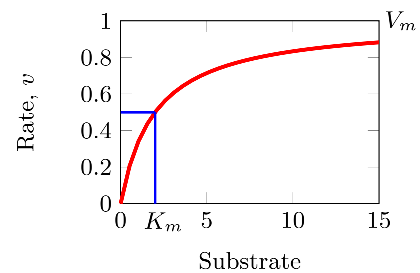
Modified Mass-Action Rate Law

$$v = k_1A\left(1 + \frac{\Gamma}{K_{eq}}\right)$$

Enzyme Rate Laws

Briggs-Haldane Rate Law:

$$v = \frac{V_mA}{A + K_m}$$



Reversible Enzymatic Rate Law

$$v = \frac{V_m}{K_{m_1}}\frac{A - B/K_{eq}}{1 + A/K_{m_1} + B/K_{m_2}}$$

Sigmoid Responses

$$v = \frac{V_mA^h}{K + A^h} \text{ Activation}$$

$$v = \frac{V_m}{K + A^h} \text{ Repression}$$

Simple Model

$A \xrightarrow{v_1} B \xrightarrow{v_2} C$

The system of differential equation for this linear chain of reactions is given by:

$$\frac{dA}{dt} = -v_1 \quad \frac{dB}{dt} = v_1 - v_2 \quad \frac{dC}{dt} = v_2$$

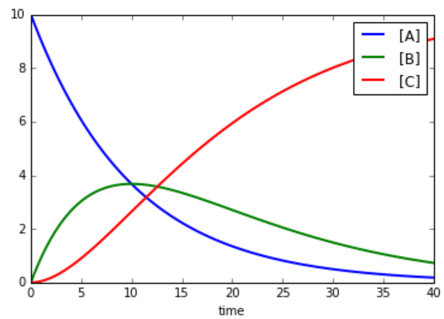
Assuming simple irreversible mass-action kinetics the model can be rewritten as:

$$\frac{dA}{dt} = -k_1 A$$

$$\frac{dB}{dt} = k_1 A - k_2 B$$

$$\frac{dC}{dt} = k_2 B$$

If we assign a value of 0.1 to both rate constants and an initial concentration of 10 units to A then a simulation of this system will yield:



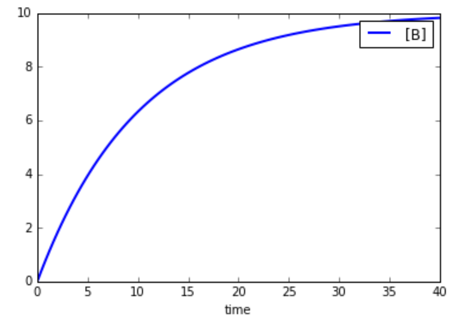
Note how all the mass of the system drains from A to C so that at the end of the simulation there is no A left.

Boundary Species

Species that do not change in time are called fixed species or boundary species. Often these species are where mass enters and leaves the system. For example is model where Glucose is used, we may consider the concentration of Glucose to be fixed over the duration of the study.

$$\boxed{A} \longrightarrow B \longrightarrow \boxed{C}$$

Note how the concentration of B now approaches steady state.



Steady State

When all species levels are unchanging, solution to:

$$\frac{dX}{dt} = 0$$

Resources

http://libroadrunner.org/
http://antimony.sourceforge.net/
http://tellurium.analogmachine.org/