

# Mass Action Reactions

Reaction	Description or Expansion
$\emptyset \rightarrow X$	Creation (introduction)
$X \rightarrow \emptyset$	Annihilation (removal)
$p_1 A_1 + p_2 A_2 + \dots \rightarrow q_1 B_1 + q_2 B_2 + \dots$	Standard mass action with stoichiometry
$A \rightleftharpoons B$	$\begin{cases} A \rightarrow B \\ B \rightarrow A \end{cases}$
$p_1 A_1 + p_2 A_2 + \dots \rightleftharpoons q_1 B_1 + q_2 B_2 + \dots$	$\begin{cases} p_1 A_1 + \dots \rightarrow q_1 B_1 + \dots \\ q_1 B_1 + \dots \rightarrow p_1 A_1 + \dots \end{cases}$
Representation of $A + X \rightleftharpoons A_X \rightleftharpoons B + X$	
$A \xrightleftharpoons{X} B$	$\begin{cases} A + X \rightarrow A_X \\ A_X \rightarrow A + X \\ A_X \rightarrow B + X \\ B + X \rightarrow A_X \end{cases}$
Representation of $A + X \rightleftharpoons A_X \rightleftharpoons B_X \rightleftharpoons B + X$	
$A \xrightleftharpoons{X} B$	$\begin{cases} A + X \rightarrow A_X \\ A_X \rightarrow A + X \\ A_X \rightarrow B_X \\ B_X \rightarrow A_X \\ B_X \rightarrow B + X \\ B + X \rightarrow B_X \end{cases}$
Typical Cascades	
$A_1 \rightarrow A_2 \rightarrow A_3 \dots$	$\begin{cases} A_1 \rightarrow A_2 \\ A_2 \rightarrow A_3 \\ \vdots \end{cases}$
$A_1 \rightleftharpoons A_2 \rightleftharpoons A_3 \dots$	$\begin{cases} A_1 \rightleftharpoons A_2 \\ A_2 \rightleftharpoons A_3 \\ \vdots \end{cases}$
$A_1 \rightleftharpoons A_2 \xrightleftharpoons{X} A_3 \dots$	$\begin{cases} A_1 \xrightleftharpoons{X} A_2 \\ A_2 \rightleftharpoons A_3 \\ \vdots \end{cases}$
$A_1 \rightleftharpoons A_2 \xrightleftharpoons{\{X_1, X_2, \dots\}} A_3 \dots$	$\begin{cases} A_1 \xrightleftharpoons{X_1} A_2 \\ A_2 \xrightleftharpoons{X_2} A_3 \\ \vdots \end{cases}$

## Michaelis-Menten-Henri Style Reactions

Syntax $\{A \implies B, \text{MM}[K, v]\}$ or $\{A \xrightarrow{x} B, \text{MM}[K, v]\}$	
$A \implies B$	$[B]' = \frac{v[A]}{K + [A]} = -[A]'$
$A \xrightarrow{x} B$	$[B]' = \frac{v[A][X]}{K + [A]} = -[A]'$
$A \rightleftharpoons B$	$[B]' = \frac{v_A[A]}{K_A + [A]} - \frac{v_B[B]}{K_B + [B]} = -[A]'$
$A \xrightleftharpoons[Y]{X} B$	$[B]' = \frac{v_A[A][X]}{K_A + [A]} - \frac{v_B[B][Y]}{K_B + [B]} = -[A]'$
Syntax $\{A \implies B, \text{MM}[k_1, k_2, k_3]\}$ or $\{A \xrightarrow{x} B, \text{MM}[k_1, k_2, k_3]\}$	
$A \implies B$	$[B]' = \frac{k_1[A]}{\frac{k_2+k_3}{k_1} + [A]} = -[A]'$
$A \xrightarrow{x} B$	$[B]' = \frac{k_1[A][X]}{\frac{k_2+k_3}{k_1} + [A]} = -[A]'$
Cascades	
$A_1 \implies A_2 \implies A_3 \implies \dots$	$\begin{cases} A_1 \implies A_2 \\ A_2 \implies A_3 \\ \vdots \end{cases}$
$A_1 \implies A_2 \xrightarrow{x} A_3 \implies \dots$	$\begin{cases} A_1 \xrightarrow{x} A_2 \\ A_2 \xrightarrow{x} A_3 \\ \vdots \end{cases}$
$A_1 \implies A_2 \xrightarrow{\{x_1, x_2, \dots\}} A_3 \implies \dots$	$\begin{cases} A_1 \xrightarrow{x_1} A_2 \\ A_2 \xrightarrow{x_2} A_3 \\ \vdots \end{cases}$

## Regulatory Hill Functions

Syntax $\{A \mapsto B, \text{hill}[v, n, K, b, T]\}$	
$A \mapsto B$	$[B]' = \frac{v(b + T[A])^n}{K^n + (b + T[A])^n}$ and $[A]' = 0$
Syntax $\{A_1 + A_2 + \dots \mapsto B, \text{hill}[v, n, K, b, \{T_1, T_2, \dots\}]\}$	
$A_1 + A_2 + \dots \mapsto B$ or $\{A_1, A_2, A_3, \dots\} \mapsto B$ or $\begin{cases} A_1 \mapsto B \\ A_2 \mapsto B \\ A_3 \mapsto B \\ \vdots \end{cases}$	$[B]' = \frac{v(b + T_1[A_1] + T_2[A_2] + \dots)^n}{K^n + (b + T_1[A_1] + T_2[A_2] + \dots)^n}$  $[A_1]' = [A_2]' = \dots = 0$

## Catalytic Hill Functions

Syntax $\{A \xrightarrow{X} B, \text{hill}[v, n, K, b, T]\}$	
$A \xrightarrow{X} B$	$[B]' = \frac{v[X](b + T[A])^n}{K^n + (b + T[A])^n} = -[A]'$
Syntax $\{A_1 + A_2 + \dots \mapsto B, \text{hill}[v, n, K, b, \{T_1, T_2, \dots\}]\}$	
$A_1 + A_2 + \dots \xrightarrow{X} B$ or $\{A_1, A_2, A_3, \dots\} \xrightarrow{X} B$ or $\begin{cases} A_1 \xrightarrow{X} B \\ A_2 \xrightarrow{X} B \\ A_3 \xrightarrow{X} B \\ \vdots \end{cases}$	$[B]' = \frac{v[X](b + T_1[A_1] + T_2[A_2] + \dots)^n}{K^n + (b + T_1[A_1] + T_2[A_2] + \dots)^n}$  $[A_1]' = [A_2]' = \dots = -[B]'$

## Logistic Rate Functions

Syntax $\{A \mapsto B, \text{GRN}[v, \beta, n, h]\}$	
$A \mapsto B$	$[B]' = \frac{v}{1 + e^{-h - \beta[A]^n}}$ $[A]' = 0$
Syntax $\{A_1 + A_2 + \dots \mapsto B, \text{GRN}[v, \{\beta_1, \beta_2, \dots\}, \{n_1, n_2, \dots\}, h]\}$	
$A_1 + A_2 + \dots \mapsto B$ or $\{A_1, A_2, \dots\} \mapsto B$ or $\begin{cases} A_1 \rightarrow B \\ A_2 \rightarrow B \\ \vdots \end{cases}$	$[B]' = \frac{v}{1 + e^{-h - \beta_1[A_1]^{n_1} - \beta_2[A_2]^{n_2} - \dots}}$ $[A_1]' = [A_2]' = \dots = 0$

## S-System Rate Functions (Synergistic Systems)

Syntax $\{A \mapsto B, \text{SSystem}[\tau, K_+, K_-, c_+, c_-]\}$	
$A \mapsto B$	$[B]' = \frac{1}{\tau} (K_+[A]^{c_+} - K_-[A]^{c_-})$ $[A]' = 0$
Syntax $\{A_1 + A_2 + \dots \mapsto B, \text{SSystem}[\tau, K_+, K_-, \{p_1, p_2, \dots\}, \{m_1, m_2, \dots\}]\}$	
$A_1 + A_2 + \dots \mapsto B$ or $\{A_1, A_2, \dots\} \mapsto B$ or $\begin{cases} A_1 \rightarrow B \\ A_2 \rightarrow B \\ \vdots \end{cases}$	$[B]' = \frac{K_+[A_1]^{p_1}[A_2]^{p_2} \dots - K_-[A_1]^{m_1}[A_2]^{m_2} \dots}{\tau}$ $[A_1]' = [A_2]' = \dots = 0$

## NHCA Rate Function (Non-Hierarchical Cooperative Activation)

Syntax $\{A \mapsto B, \text{NHCA}[\nu, \{\alpha, \beta\}, n, m, k]\}$	
$A \mapsto B$	$[B]' = \frac{\nu(1 + \alpha[A]^n)^m}{(1 + \alpha[A]^n)^m + k(1 + \beta[A]^n)^m}$ $[A]' = 0$
Syntax $\{A_1 + A_2 + \dots \mapsto B, \text{NHCA}[\nu, \{\{\alpha_1, \beta_1\}, \{\alpha_2, \beta_2\}, \dots\}, \{n_1, n_2, \dots\}, m, k]\}$ Syntax $\{A_1 + A_2 + \dots \mapsto B, \text{NHCA}[\nu, \{\{\alpha_1, \beta_1\}, \{\alpha_2, \beta_2\}, \dots\}, n, m, k]\}$	
$A_1 + A_2 + \dots \mapsto B$ or $\{A_1, A_2, \dots\} \mapsto B$ or $\begin{cases} A_1 \mapsto B \\ A_2 \mapsto B \\ \vdots \end{cases}$	$[B]' = \frac{\nu \prod_j (1 + \alpha_j [A_j]^{n_j})^m}{\prod_j (1 + \alpha_j [A_j]^{n_j})^m + k \prod_j (1 + \beta_j [B_j]^{n_j})^m}$ $[A_1]' = [A_2]' = \dots = 0$
Syntax $\{A \mapsto B, \text{NHCA}[\nu, T, n, m, k]\}$ Syntax $\{A_1 + A_2 + \dots \mapsto B, \text{NHCA}[\nu, \{T_1, T_2, \dots\}, \{n_1, n_2, \dots\}, m, k]\}$	
$A \mapsto B$	$[B]' = \frac{\nu(1 + T\mathcal{U}(T)[A]^n)^m}{(1 + T\mathcal{U}(T)[A]^n)^m + k(1 + T\mathcal{U}(-T)[A]^n)^m}$ $[A]' = 0$
$A_1 + A_2 + \dots \mapsto B$ or $\{A_1, A_2, \dots\} \mapsto B$ or $\begin{cases} A_1 \mapsto B \\ A_2 \mapsto B \\ \vdots \end{cases}$	$[B]' = \frac{\nu \prod_j (1 + T_j \mathcal{U}(T_j)[A_i]^{n_j})^m}{\prod_j (1 + T_j \mathcal{U}(-T_j)[A_j]^{n_j})^m + k \prod_j (1 + T_j \mathcal{U}(-T_j)[A_j]^{n_j})^m}$ $[A_1]' = [A_2]' = \dots = 0$

## MWC/GWMC Rate Function (Generalized Monod-Wyman-Changeaux)

Syntax $\{A \xrightarrow{X} B, \text{MWC}[\mathbf{k}_{\text{cat}}, \mathbf{n}, \mathbf{c}, \ell, \mathbf{K}]\}$	
$A \xrightarrow{X} B$	$[B]' = k_{\text{cat}}[X] \frac{\alpha(1+\alpha)^{n-1} + c\ell\alpha(1+c\alpha)^{n-1}}{(1+\alpha)^n + \ell\alpha(1+c\alpha)^n}$ where $\alpha = \frac{[A]}{K}$ $[A]' = -[B]'$
$S \xrightarrow{X} P$ $\{\mathbf{A}, \mathbf{I}\}$	$[B]' = k_{\text{cat}}[X] \frac{s(1+s)^{n-1} + cLs(1+cs)^{n-1}}{(1+s)^n + Ls(1+cs)^n}$ with $L = \left(\frac{1+i}{1+a}\right)^n$ , $\ell = \frac{[S]}{K}$ , $i = \frac{[I]}{K_I}$ , $a = \frac{[A]}{K_A}$ $[A]' = -[B]'$
Syntax $\{\{\mathbf{S}_1, \mathbf{S}_2, \dots\} \xrightarrow{X} \{\mathbf{P}_1, \mathbf{P}_2, \dots\}, \text{MWC}[\{\mathbf{k}_1, \mathbf{k}_2, \dots\}, \mathbf{n}, \mathbf{c}, \ell, \mathbf{K}]\}$ $\{\{\mathbf{A}_1, \mathbf{A}_2, \dots\}, \{\mathbf{I}_1, \mathbf{I}_2, \dots\}\}$	
$[P_q]' = k_q[X] \frac{\prod_i (1+a_i)^n \prod_j (1+s_j)^{n-1} \prod_k s_k + \ell \prod_i (cs_i) \prod_j (1+cs_j)^{n-1} \prod_k (1+i_k)^n}{\prod_i (1+a_i)^n \prod_j (1+s_j)^n + \ell \prod_i (1+cs_i)^{n-1} \prod_j (1+i_j)^n}$ where $s_j = \frac{[S_j]}{K_{S_j}}$ , $a_j = \frac{[A_j]}{K_{A_j}}$ , $i_j = \frac{[I_j]}{K_{I_j}}$	
Syntax $\{\{\mathbf{S}_1, \mathbf{S}_2, \dots\} \xrightarrow{X} \{\mathbf{P}_1, \mathbf{P}_2, \dots\}, \text{MWC}[\{\mathbf{k}_1, \mathbf{k}_2, \dots\}, \mathbf{n}, \mathbf{c}, \ell, \mathbf{K}]\}$ $\{\{\mathbf{A}_1, \mathbf{A}_2, \dots\}, \{\mathbf{I}_1, \mathbf{I}_2, \dots\}\}, \{\{\mathbf{C}'_{11}, \mathbf{C}'_{12}, \dots\}, \{\mathbf{C}'_{21}, \mathbf{C}'_{22}, \dots\}, \dots, \{\mathbf{A}'_{11}, \mathbf{A}'_{12}, \dots\}, \dots\}$ here $C_{j1}, C_{j2}, \dots$ are competitive inhibitors of $S_j$ , $A'_{i1}, A'_{i2}, \dots$ are competitive activators of $A_i$	
$[P_q]' = \frac{\prod_i (1+a_i + \bar{a}_i)^n \prod_j (1+s_j + \bar{s}_j)^{n-1} \prod_m s_m + L \prod_i (cs_i) \prod_j (1+cs_j + c\bar{s}_j)^{n-1} + \prod_m (1+i_m)^n}{\prod_i (1+a_i + \bar{a}_i)^n \prod_j (1+s_j)^n + L \prod_j (1+cs_j + c\bar{s}_j)^{n-1} + \prod_m (1+i_m)^n}$ where $s_j = \frac{[S_j]}{K_{S_j}}$ , $a_j = \frac{[A_j]}{K_{A_j}}$ , $i_j = \frac{[I_j]}{K_{I_j}}$ , $\bar{s}_j = \sum_q \frac{[C_{jq}]}{K_{S_{jq}}}$ , $\bar{a}_j = \sum_q \frac{[A'_{jq}]}{K_{A'_{jq}}}$	

## Rational Function Rate Law

$\{\{\{A_1, A_2, \dots\}, \{B_1, B_2, \dots\}\} \Rightarrow X$ $\text{rational}\{\{a_0, \dots\}, \{b_0, \dots\}, \{p_1, \dots\}, \{q_1, \dots\}\}$
$[X]' = \frac{a_0 + a_1[A_1]^{p_1} + a_2[A_2]^{p_2} + \dots}{b_0 + b_1[B_1]^{q_1} + b_2[B_2]^{q_2} + \dots}$ $[A_1]' = [A_2]' = \dots = [B_1]' = [B_2]' = \dots = 0$

## User-Defined Stoichiometric Rate Laws

Syntax $\{p_1A_1 + p_2A_2 + \dots \Rightarrow q_1B_1 + q_2B_2 + \dots, f[A_1[t], A_2[t], \dots, B_1[t], B_2[t], \dots]\}$
$[X_i]' = (q_i - p_i)f[A_1[t], A_2[t], \dots, B_1[t], \dots]$

## User-Defined Regulatory Rate Laws

$\{A \mapsto B, \text{name}[r, T, n, h, f]\}$	$[B]' = rf(h + T[A]^n)$
$A_1 + A_2 + \dots \mapsto B$ or $\{A_1, A_2, \dots\} \mapsto B$ or $\begin{cases} A_1 \mapsto B \\ A_2 \mapsto B \\ \vdots \end{cases}$	$[B]' = rf(h + T_1[A_1]^{n_1} + T_2[A_2]^{n_2} + \dots)$

## Flux-Only Reactions

$\{p_1X_1 + p_2X_2 + \dots \rightarrow q_1Y_1 + q_2Y_2 + \dots,$ $\text{Flux}[\text{lower bounds}, \text{variable name}, \text{upper bounds}, \text{value}, \text{objective coefficient}]\}$
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