Cellerator™ Arrow Quick Reference

Cellerator Arrow	Name, `interpret[]` format, Differential Equations	Typical Biochemical Notation and other notes
$S \to P$	**Conversion**: `interpret[{{S→P,k},...]` $\frac{dP}{dt} = kS, \ \frac{dS}{dt} = -kS$	$S \xrightarrow{k} P$
$A + B \to C$	**Unidirectional**: `interpret[{{A+B→C,k},...}]` $\frac{dA}{dt} = -kAB, \ \frac{dB}{dt} = -kAB, \ \frac{dC}{dt} = kAB$	$A + B \xrightarrow{k} C$
$A + B^n \to C$	**Cooperative Unidirectional**: (n must be an integer) interpret[{{A + B^n → C,k},...}] $\frac{dA}{dt} = \frac{dB}{dt} = -kAB^n = -\frac{dC}{dt}$	$A + nB \xrightarrow{k} C$
$A \rightleftarrows B$	**Bidirectional Conversion:** `interpret[{{A ⇄ B, kf, kr}, ...}]` $\frac{dA}{dt} = -\frac{dB}{dt} = -k_f A + k_r B,$	$A \underset{k_r}{\overset{k_f}{\rightleftarrows}} B$
$A + B \rightleftarrows C$	**Bidirectional**: `interpret[{{A + B ⇄ C, kf, kr}, ...}]` $\frac{dA}{dt} = \frac{dB}{dt} = -\frac{dC}{dt} = -k_f AB + k_r C,$	$A + B \underset{k_r}{\overset{k_f}{\rightleftarrows}} C$
$\phi \to A$	**Creation**: `interpret[{{ϕ→A,k},...]` $\frac{dA}{dt} = k$	$\xrightarrow{k} A$
$A \to \emptyset$	**Annihilation**: `interpret[{{A → ∅, k}, ...}]` $\frac{dA}{dt} = -kA$	$A \xrightarrow{k}$
$S \overset{E}{\rightleftarrows} P$	**Catalytic***: interpret$\left[\left\{\left\{S \overset{En}{\rightleftarrows} P,\ kf,\ kr,\ k\right\},\ ...\right\}\right]$ $\frac{dS}{dt} = -k_f SE + k_r X, \ \frac{dP}{dt} = kX,$ $\frac{dX}{dt} = -\frac{dE}{dt} = k_f SE - (k + k_r)X$	$S + E \underset{k_r}{\overset{k_f}{\rightleftarrows}} X \xrightarrow{k} E + P$
$S \underset{F}{\overset{E}{\rightleftarrows}} P$	**Bidirectional Catalytic***: interpret$\left[\left\{\left\{A \underset{F}{\overset{En}{\rightleftarrows}} B,\ a1,\ d1,\ k1,\ a2,\ d2,\ k2\right\},\right.\right.$ $\frac{dS}{dt} = a_1 SE + d_1 X + k_2 Y, \ \frac{dP}{dt} = k_1 X - a_2 PF + d_2 Y$ $\frac{dE}{dt} = -a_1 SE + (d_1 + k_1)X = -\frac{dX}{dt},$ $\frac{dF}{dt} = -a_2 PF + (d_2 + k_2)Y = -\frac{dY}{dt}$	$S + E \underset{d_1}{\overset{a_1}{\rightleftarrows}} X \xrightarrow{k_1} E + P$ $P + F \underset{d2}{\overset{a2}{\rightleftarrows}} Y \xrightarrow{k_2} F + S$ Equivalent to the set $\left\{S \overset{E}{\rightleftarrows} P,\ P \overset{F}{\rightleftarrows} S\right\}$
$S \overset{E}{\to} P$	**Simplifed non-saturating catalytic***: interpret$\left[\left\{\left\{S \overset{En}{\to} P,\ k\right\},\ ...\right\}\right]$ $\frac{dP}{dt} = kES, \ \frac{dS}{dt} = -kES$	$S + E \xrightarrow{k} P + E$

Cellerator Arrow	Name, `interpret[]` format, Differential Equations	Typical Biochemical Notation and other notes

$S \overset{E}{\mapsto} P$	**Simplified Saturating Catalytic***:
	`interpret[{{A↦B,hill[options]},...}]`
	$\frac{dP}{dt}=\frac{(k_0+kE)S}{K_M+S}$, $\frac{dS}{dt}=\frac{-(k_0+kE)S}{K_M+S}$
	`Options[hill]={vmax→1,nhill→1,khalf→1,basalRate→0}`
	In this example: `vmax` $\to k$, `basalRate` $\to k_0$, `khalf` $\to K_M$, `nhill` $\to n$
	* The variable "E" is used for illustrative purposes only, and should be avoided. Mathematica assigns a value of 2.718… to the symbol E.
		Gives Michaelis-Menten kinetics when $k_0=0$.
		Equivalent to $S \overset{E}{\rightleftarrows} P$ under the assumptions that (1) the concentration of intermediate (X) is steady state; (2) that E represents total (free plus bound) enzyme, (3) that $K_M=(k+k_r)/k_f$, and (4) the basal rate $k_0=0$.

$A \mapsto B$	**Transcriptional regulation** of B by A:
	`interpret[{{A↦B,hill[options]},...}]`
	$\frac{dB}{dt}=r_0+\frac{r_1+vA^n}{k^n+A^n}$, $\frac{dA}{dt}=0$
	`Options[hill]={vmax→1,nhill→1,khalf→1,basalRate→0}`
	In this example: `vmax` $\to v$, `basalRate` $\to \{r_0,r_1\}$, `khalf` $\to K_M$, `nhill` $\to n$
	If `basalRate` is an Atom it is used for r_0 and $r_1=0$
		The set $\{A_i \mapsto B\}$, $i=1,2,\ldots,p$, is interpreted as:
		$$\frac{dB}{dt}=r_0+\frac{\left(r_1+\sum_{i=1}^{p} v_i T_i A_i\right)^n}{k^n+\left(r_1+\sum_{i=1}^{p} v_i T_i A_i\right)^n}$$

$A \mapsto B$	**Transcriptional Regulation** of B by A:
	`interpret[{{A↦B,GRN[options]},...}]`
	$\frac{dB}{dt}=\frac{R}{1+e^{-TA^n+h}}$
	`Options[GRN]={RGRN→1,TGRN→1,nGRN→1,hGRN→0}`
	In this example, `RGRN` $\to R$, `TGRN` $\to T$, `nBRN` $\to n$, `hGRN` $\to h$
		The set $\{A_i \mapsto B\}$, $i=1,2,\ldots,p$, is interpreted as:
		$$\frac{dB}{dt}=\frac{R}{1+e^{-\left(\sum_i T_i A_i^{n_i}+h_i\right)}}$$

$A \mapsto B$	**NHCA dynamics***, regulation of B by A:
	`interpret[{{A↦B,NHCA[options]},...}]`
	$\frac{dB}{dt}=\frac{(1+T^+A^n)^m}{k(1+T^-A^n)^m+(1+T^+A^n)^m}$, or,
	$\frac{dB}{dt}=\frac{(1+T\Theta(T)A^n)^m}{k(1-T\Theta(-T)A^n)^m+(1+T\Theta(T)A^n)^m}$
	`Options[NHCA]={TPLUS→1,TMINUS→1,nNHCA→1,kNHCA→1,mNHCA→1,TNHCA→{}}`
	If `TMCW` is anything besides {} then the second form of the equation is used. If `TMCW` is not specified then the system defaults to the first equation.
	In the first example, `TPLUS` $\to T^+$, `TMINUS` $\to T^-$, `nNHCA` $\to n$, `mNHCA` $\to m$, `kNHCA` $\to k$
	In the second example, `TNHCA` $\to T$, `nNHCA` $\to n$, `mNHCA` $\to m$, `kNHCA` $\to k$
	* Non-Heirarchical Cooperative Activation. The (+) and (-) in the superscript are used for illustrative purposes only here; they will lead to confusion in Mathematica and should be avoided.
		The set $\{A_i \mapsto B\}$, $i=1,2,\ldots,p$, is interpreted as:
		$$\frac{dB}{dt}=\frac{\prod_i(1+T_i^+A_i^{n_i})^m}{k\prod_i(1+T_i^-A_i^{n_i})^m+\prod_i(1+T_i^+A_i^{n_i})^m}$$, or
		$$\frac{dB}{dt}=\frac{\prod_i(1+T_i\Theta(T_i)A_i^{n_i})^m}{k\prod_i(1-T_i\Theta(-T_i)A_i^{n_i})^m+\prod_i(1+T_i\Theta(T_i)A_i^{n_i})^m}$$

$\langle A_1,A_2,\ldots\rangle \mapsto C$	**NHCA dynamics with Competitive Binding.** `interpret[{{A↦B,NHCA[options]},...}]`
	`Options[NHCA]={TPLUS→{TP1,TP2,...},TMINUS→{TM1,TM2,...},nNHCA→{n1,n2,...},kNHCA→1`
	`mNHCA→1,TNHCA→{}}`
	$\frac{dC}{dt}=\left\{1+\left(\sum_i T_i^+A_i^{n_i}\right)^m\right\}\Big/\left\{k\left(\sum_i T_i^-A_i^{n_i}\right)^m+\left(\sum_i T_i^+A_i^{n_i}\right)^m\right\}$
	$\frac{dC}{dt}=\left\{1+\left(\sum_i T_i\Theta(T_i)A_i^{n_i}\right)^m\right\}\Big/\left\{k\left(\sum_i(-T_i)\Theta(-T_i)A_i^{n_i}\right)^m+\left(\sum_i T_i\Theta(T_i)A_i^{n_i}\right)^m\right\}$ if `TNHCA` $\to$ `{T1,T2,...}` $\neq$ `{}`	