Reactor Specifications

The E-Cell Project

March 2, 2000

Contents

1 CatalyzedMassActionReactor

Classname	CatalyzedMassActionReactor
Base Class	FluxReactor
Brief Description	Reaction rate directory depends on the concentrations of the catalyst and substances

Version				Date
E-CELL	ecs-v09	Reactor	0.1	29/6/1999

Author	Kouichi Takahashi
E-mail	shafi@sfc.keio.ac.jp

Description
A reactor class in which general mass action equation is embeded. A 'catalyst' is defined as a molecular species that doesn't change itself but has effect on reaction rate following general mass action low. Velocity is calculated as a product of concentrations of the catalyst and substrates, and a kinetic constant (see Equation).

Equation
$$v = k \prod_{i=0}^{n} [S_i]^{c_i}$$

Substance	Max	Min	Remarks
Substrate	Inf	1	
Product	Inf	1	
Catalyst	1	1	

Parameter	Type	Unit	Description
k	Float		Velocity Constant

Notes

2 ConstantParameterReactor

Classname	ConstantParameterReactor
Base Class	Reactor
Brief Description	Sets constant parameter

Version				Date
E-CELL	ecs-v08	Reactor	0.1	18/7/1999

Author	Yusuke Saito
E-mail	t96406ys@sfc.keio.ac.jp

Description
A reactor class which simply substitutes certain unchanged value for a parameter. For example, this reactor offers handiness of setting volume value of a certain system of which volume assumed to be unchanged during simulation. !!!It is indispensable for simulation to set volume value of any system (which is designed to have one) at THE FIRST STEP of the simulation. So, you must set 'InitialActivity' of this reactor in case of using it to set volume value. Or, volume value of the system set to zero(default) and cause floating exception.

Equation
Parameter

Substance	Max	Min	Remarks

Parameter	Type	Unit	Description
Value	Float		Parameter

Notes

3 DecayReactor

Classname	DecayReactor
Base Class	FluxReactor
Brief Description	Disintegration or decay process.

Version				Date
E-CELL	ecs-v08	Reactor	0.1	29/6/1999

Author	Kouichi Takahashi
E-mail	shafi@sfc.keio.ac.jp

Description
A reactor class for disintegration or decay processes. The quantity of the 'Substrate' is reduced according to the half-life inputted.

Equation
$$S(t) = S(0)e^{-\frac{ln2}{T}t}$$

Substance	Max	Min	Remarks
Substrate	1	1	
Product	Inf	0	
Catalyst	0	0	
Effector	0	0	

Parameter	Type	Unit	Description
T	Float		Half Time

Notes
MassActionReactor: $k = \frac{ln2}{T}$

4 GeneralRapidEquilibriumPReactor

Classname	GeneralRapidEquilibriumPReactor
Base Class	Reactor
Brief Description	Solver of Algebraic Equation of a pathway which rapidlly reaches equilibrium

Version				Date
E-CELL	ecs-1.0	Reactor	0.1	2000 2/2

Author	Kenta Hashimoto
E-mail	kem@sfc.keio.ac.jp

Description
A reactor class for pathways which rapidly (within a step) reaches a state of equilibrium. This reactor calculates velocity according to the equilibrium constant inputted by the user. In case that substrates are already at a state of equilibrium, velocity is set to zero.

Equation
$$k_{eq} \prod([S_k] - v) = \prod([P_k] + v)$$

Substance	Max	Min	Remarks
Substrate	inf	1	
Product	inf	1	

Parameter	Type	Unit	Description
Precision	Float		precision
Keq0	Float	M	Equilibrium constant
Keq1	Float	M	Equilibrium constant
Keq2	Float	M	Equilibrium constant
Keq3	Float	M	Equilibrium constant
Keq4	Float	M	Equilibrium constant
Keq5	Float	M	Equilibrium constant
Keq6	Float	M	Equilibrium constant
Keq7	Float	M	Equilibrium constant
Keq8	Float	M	Equilibrium constant
Keq9	Float	M	Equilibrium constant
Keq10	Float	M	Equilibrium constant
Keq11	Float	M	Equilibrium constant
Keq12	Float	M	Equilibrium constant
Keq13	Float	M	Equilibrium constant
Keq14	Float	M	Equilibrium constant
Keq15	Float	M	Equilibrium constant
Keq16	Float	M	Equilibrium constant
Keq17	Float	M	Equilibrium constant
Keq18	Float	M	Equilibrium constant
Keq19	Float	M	Equilibrium constant

Notes
"v" is velosity.

5 IsoUniUniReactor

Classname	IsoUniUniReactor
Base Class	FluxReactor
Brief Description	Iso Uni Uni Reaction system

Version				Date
E-CELL	ecs-v08	Reactor	0.1	29/6/1999

Author	Yusuke Saito
E-mail	t96406ys@sfc.keio.ac.jp

Description

This reactor is applicable to Iso Uni Uni sequence which is uncommon in ordinary soluble enzyme systems but can approximate membrane transport systems.
Reaction sequence considered here is:

$$E + S \rightleftharpoons^{k_1}_{k_{-1}} ES \rightleftharpoons^{k_2}_{k_{-2}} E'P \rightleftharpoons^{k_3}_{k_{-3}} P + E'$$

$$E' \rightleftharpoons^{k_4}_{k_{-4}} E$$

where, for example,

E	binding protein or carrier molecule
S	external substrate
ES	ES complex
E'P	comformationally or locationally changed ES
P	intracellular substrate
E'	free E which can not immediately access to S

Velocity is derived algebraically from steady-state assumptions and the equation is derived using the schematic method of King and Altman.

Equation

$$v = \frac{K_{cF}[E]([S] - \frac{[P]}{K_{eq}})}{K_{mS}(1 + \frac{[P]}{K_{mP}}) + [S](1 + \frac{[P]}{K_{iip}})}$$

Substance	Max	Min	Remarks
Substrate	1	1	
Product	1	1	
Catalyst	1	1	
Effector	0	0	

Parameter	Type	Unit	Description
KcF	Float		Catalytic Constant (Forward)
KmS	Float		Michaelis Constant of Substrate S
KmP	Float		Michaelis Constant of Product P
Keq	Float		Equibrium Constant
KiiP	Float		Iso Inhibition Constant of Product P

Notes
Isomerization E - E'

6 MassActionReactor

Classname	MassActionReactor
Base Class	FluxReactor
Brief Description	General Mass Action

Version				Date
E-CELL	ecs-v09	Reactor	0.1	29/6/1999

Author	Kouichi Takahashi
E-mail	shafi@sfc.keio.ac.jp

Description
A reactor class in which general mass action equation is embeded. Velocity is calculated as a product of concentrations of substrates and a kinetic constant (see Equation). General mass action law is generally applicable to simple kinetic processes such as elementary reaction and other processes in which its velocity is directly propotional to their substrates.

Equation
$$v = k \prod_{i=0}^{n} [S_i]^{c_i}$$

Substance	Max	Min	Remarks
Substrate	inf	1	
Product	inf	1	
Catalyst	0	0	
Effector	0	0	

Parameter	Type	Unit	Description
k	Float		Velocity Constant

Notes

7 MichaelisUniUniReactor

Classname	MichaelisUniUniReactor
Base Class	FluxReactor
Brief Description	Unireactant enzyme activity of which kinetics can be described by Henri-Michaelis-Menten equation

Version				Date
E-CELL	ecs-v09	Reactor	0.1	29/6/1999

Author	Yusuke Saito
E-mail	t96406ys@sfc.keio.ac.jp

Description

A reactor class for unireactant enzyme activity of which kinetics can be described by Henri-Michaelis-Menten equation derived from rapid equilibrium assumptions.

This reactor is applicable to reaction visualized as:

$$E + S \rightleftharpoons_{k_{-1}}^{k_1} ES \rightarrow^{k_p} E + P$$

Equation

$$v = \frac{K_{cF}[E][S]}{K_{mS} + [S]}$$

Substance	Max	Min	Remarks
Substrate	1	1	
Product	1	1	
Catalyst	1	1	
Effector	0	0	

Parameter	Type	Unit	Description
KmS	Float	mol/l	Michaelis Constant of Substrate
KcF	Float	1/s	Catalystic Constant

Notes

8 MichaelisUniUniReversibleReactor

Classname	MichaelisUniUniReversibleReactor
Base Class	FluxReactor
Brief Description	Reversible, unireactant enzyme activity of which kinetics can be described by Henri-Michaelis-Menten equation

Version				Date
E-CELL	ecs-v09	Reactor	0.1	29/6/1999

Author	Yusuke Saito
E-mail	t96406ys@sfc.keio.ac.jp

Description

A reactor class for reversible, unireactant enzyme activity of which kinetics can be described by Henri-Michaelis-Menten equation.

This reactor is applicable to reaction visualized as:

$$E + S \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} ES \underset{k_{-2}}{\overset{k_2}{\rightleftharpoons}} E + P$$

Assuming only one central complex, [ES], the net velocity in the forward direction is given by:

$$V_{net} = k_2[ES] - k_{-2}[E][P] \qquad \text{(for solved form, see Equation)}$$

Equation

$$v = \frac{(K_{cF}K_{mP}[S] - K_{cR}K_{mS}[P])[E]}{K_{mS}[P] + K_{mP}[S] + K_{mS}K_{mP}}$$

Substance	Max	Min	Remarks
Substrate	1	1	
Product	1	1	
Catalyst	1	1	
Effector	0	0	

Parameter	Type	Unit	Description
KmS	Float	mol/l	Michaelis Constant of Substrate
KmP	Float	mol/l	Michaelis Constant of Product
KcF	Float	1/s	Catalytic Constant (Forward)
KcR	Float	1/s	Catalytic Constant (Reverse)

Notes

9 OrderedBiBiReactor

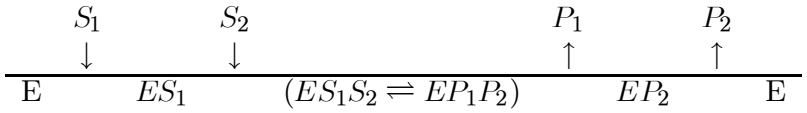
Classname	OrderedBiBiReactor
Base Class	FluxReactor
Brief Description	Ordered Bi Bi reaction system

Version				Date
E-CELL	ecs-v08	Reactor	0.2	29/6/1999

Author	Yusuke Saito
E-mail	t96406ys@sfc.keio.ac.jp

Description

A reactor class for ordered reaction that is bireactant in both direction which can be written using the Cleland notation as follows:



Velocity is derived algebraically from steady-state assumptions and the equation is derived using the schematic method of King and Altman.

Equation

Substance	Max	Min	Remarks
Substrate	2	2	
Product	2	2	
Catalyst	1	1	

Parameter	Type	Unit	Description
KcF	Float		Catalytic Constant (Forward)
KcR	Float		Catalytic Constant (Reverse)
Keq	Float		Equibrium Constant
KmS1	Float		Michaelis Constant of Substrate S1
KmS2	Float		Michaelis Constant of Substrate S2
KmP1	Float		Michaelis Constant of Product P1
KmP2	Float		Michaelis Constant of Produce P2
KiS1	Float		Inhibition Constant of Substrate S1
KiS2	Float		Inhibition Constant of Substrate S2
KiP1	Float		Inhibition Constant of Product P1
KiP2	Float		Inhibition Constant of Product P2

Notes

10 OrderedBiUniReactor

Classname	OrderedBiUniReactor
Base Class	FluxReactor
Brief Description	Ordered Bi Uni reaction system

Version				Date
E-CELL	ecs-v09	Reactor	0.1	29/6/1999

Author	Yusuke Saito
E-mail	t96406ys@sfc.keio.ac.jp

Description

A reactor class for Ordered Uni Bi sequence which can be written:

$$E + S_1 \rightleftharpoons^{k_1}_{k_{-1}} S_2 + ES_1 \rightleftharpoons^{k_2}_{k_{-2}} (ES_1S_2 \rightleftharpoons EP) \rightleftharpoons^{k_3}_{k_{-3}} E + P$$

Since the isomerization of the central complex has no effect on the final form of the velocity equation, we can combine ES_1S_2 and EP.
Velocity is derived algebraically from steady-state assumptions and the equation is derived using the schematic method of King and Altman.

Equation

$$v = \frac{K_{cF}K_{cR}[E]([P] - \frac{[A][B]}{K_{eq}})}{K_{cF}K_{mP} + K_{cF}[B] + \frac{K_{cR}K_{mA}[B]}{K_{eq}} + \frac{K_{cR}K_{mB}[A]}{K_{eq}} + \frac{K_{cF}[B][P]}{K_{ib}} + \frac{K_{cF}[A][B]}{K_{eq}}}$$

Substance	Max	Min	Remarks
Substrate	2	2	
Product	1	1	
Catalyst	1	1	

Parameter	Type	Unit	Description
KcF	Float		Catalytic Constant (Forward)
KcR	Float		Catalytic Constant (Reverse)
Keq	Float		Equibrium Constant
KmS1	Float		Michaelis Constant of Substrate S1
KmS2	Float		Michaelis Constant of Substrate S2
KmP	Float		Michaelis Constant of Product P
KiS2	Float		Inhibition Constant of Substrate S2

Notes

11 OrderedUniBiReactor

Classname	OrderedUniBiReactor
Base Class	FluxReactor
Brief Description	Ordered Uni Bi reaction system

Version				Date
E-CELL	ecs-v09	Reactor	0.1	29/6/1999

Author	Yusuke Saito
E-mail	t96406ys@sfc.keio.ac.jp

Description

A reactor class for Ordered Uni Bi sequence which can be written:

$$E + S \rightleftharpoons_{k_{-1}}^{k_1} (ES \rightleftharpoons EP_1P_2) \rightleftharpoons_{k_{-2}}^{k_2} P_1 + EP_2 \rightleftharpoons_{k_{-3}}^{k_3} E + P_2$$

Since the isomerization of the central complex has no effect on the final form of the velocity equation, we can combine $ESandEP_1P_2$.
Velocity is derived algebraically from steady-state assumptions and the equation is derived using the schematic method of King and Altman.

Equation

$$v = \frac{K_{cF}K_{cR}[E]([S] - \frac{[P1][P2]}{K_{eq}})}{K_{cR}K_{mS} + K_{cR}[S] + \frac{K_{cF}K_{mP2}[P1]}{K_{eq}} + \frac{K_{cF}K_{mP1}[P2]}{K_{eq}} + \frac{K_{cR}[S][P1]}{K_{iP1}} + \frac{K_{cR}[P1][P2]}{K_{eq}}}$$

Substance	Max	Min	Remarks
Substrate	1	1	
Product	2	2	
Catalyst	1	1	

Parameter	Type	Unit	Description
KcF	Float	1/s	Catalytic Constant (Forward)
KcR	Float	1/s	Catalytic Constant (Reverse)
Keq	Float	mol/l	Equilibrium Constant
KmS	Float	mol/l	Michaelis Constant of Substrate S
KmP1	Float	mol/l	Michaelis Constant of Product P1
KmP2	Float	mol/l	Michaelis Constant of Product P2
KiP1	Float	mol/l	Inhibition Constant of Product P1

Notes

12 PingPongBiBiReactor

Classname	PingPongBiBiReactor
Base Class	FluxReactor
Brief Description	Ping Pong Bi Bi reaction system

Version				Date
E-CELL	ecs-v09	Reactor	0.1	29/6/1999

Author	Yusuke Saito
E-mail	t96406ys@sfc.keio.ac.jp

Description

A reactor class for Ping Pong reaction system in which a product is released between the addition of two substrates. Ping Pong mechanisms are common in group transfer or "substituted enzyme" reactions, for example, a transaminase reaction.
Using the Cleland notation, the reaction can be written as:

$$\begin{array}{ccccccc} & S_1 & & & P_1 & S_2 & & & P_2 \\ & \downarrow & & & \uparrow & \downarrow & & & \uparrow \\ \hline \mathrm{E} & & (ES_1 \rightleftharpoons FP_1) & & F & & (FS_2 \rightleftharpoons EP_2) & & \mathrm{E} \end{array}$$

Velocity is derived algebraically from steady-state assumptions and the equation is derived using the schematic method of King and Altman.

Equation

$$v = \frac{K_{cF}K_{cR}[E]([S1][S2] - \frac{[P1][P2]}{K_{eq}})}{K_{cR}K_{mS2}[S1] + K_{cR}K_{mS1}[S2] + \frac{K_{cF}K_{mP2}[P1]}{K_{eq}} + \frac{K_{cF}K_{mP1}[P2]}{K_{eq}} + K_{cR}[S1][S2] + \frac{K_{cF}K_{mP2}}{K_{eq}K_{}}}$$

Substance	Max	Min	Remarks
Substrate	2	2	
Product	2	2	
Catalyst	1	1	
Effector	0	0	

Parameter	Type	Unit	Description
KcF	Float		Catalytic Constant (Forward)
KcR	Float		Catalytic Constant (Reverse)
Keq	Float		Equibrium Constant
KmS1	Float		Michaelis Constant of Substrate S1
KmS2	Float		Michaelis Constant of Substrate S2
KmP1	Float		Michaelis Constant of Product P1
KmP2	Float		Michaelis Constant of Produce P2
KiS1	Float		Inhibition Constant of Substrate S1
KiP2	Float		Inhibition Constant of Product P2

Notes

13 RandomBiBiReactor

Classname	RandomBiBiReactor
Base Class	FluxReactor
Brief Description	Random Bi Bi reaction system

Version				Date
E-CELL	ecs-v09	Reactor	0.1	30/6/1999

Author	Masayuki Okayama
E-mail	t98204mo@sfc.keio.ac.jp

Description
A reactor class for a random bireactant system in the Bi Bi direction.

Equation

Substance	Max	Min	Remarks
Substrate	2	2	
Product	2	2	
Catalyst	1	1	

Parameter	Type	Unit	Description
k_1	Float		
k_{-1}	Float		
k_2	Float		
k_{-2}	Float		
k_3	Float		
k_{-3}	Float		
k_4	Float		
k_{-4}	Float		
k_5	Float		
k_{-5}	Float		
k_6	Float		
k_{-6}	Float		
k_7	Float		
k_{-7}	Float		
k_8	Float		
k_{-8}	Float		

Notes

14 RandomBiUniReactor

Classname	RandomBiUniReactor
Base Class	FluxReactor
Brief Description	Random Bi Uni reaction system

Version				Date
E-CELL	ecs-v09	Reactor	0.1	30/6/1999

Author	Masayuki Okayama
E-mail	t98204mo@sfc.keio.ac.jp

Description
A reactor class for a random bireactant system in the Bi Uni direction. Velocity is derived algebraically from steady-state assumptions and the equation is derived using the schematic method of King and Altman.

Equation

$$v = \frac{M(P)\,[E]}{Den}$$

$M(P) = k_{-1}k_{-2}k_{-5}(-k_{-3} - k_{-4})[P] + k_{+5}(k_{+1}k_{-2}k_{+3} + k_{-1}k_{+2}k_{+4})[S_1][S_2] - k_{-1}k_{-3}k_{+4}k_{-5}[S_1][P] - k_{-2}k_{+3}k_{-4}k_{-5}[S_2][P] + k_{+1}k_{+3}k_{+4}k_{+5}[S_1]^2[S_2] + k_{+2}k_{+3}k_{+4}k_{+5}[S_1][S_2]^2$

$Den = k_{-1}k_{-2}(k_{-3} + k_{-4} + k_{+5}) + (k_{+1}k_{-2}k_{-3} + k_{+1}k_{-2}k_{-4} + k_{+1}k_{-2}k_{+5} + k_{-1}k_{-3}k_{+4} + k_{-1}k_{+4}k_{+5})[S_1] + (k_{-1}k_{+2}k_{-3} + k_{-1}k_{+2}k_{-4} + k_{-1}k_{+2}k_{+5} + k_{-2}k_{+3}k_{-4} + k_{-2}k_{+3}k_{+5})[S_2] + k_{-5}(k_{-1}k_{-2} + k_{-1}k_{-4} + k_{-2}k_{-3})[P] + (k_{+1}k_{-2}k_{+3} + k_{+1}k_{+3}k_{-4} + k_{-1}k_{+2}k_{+4} + k_{+2}k_{-3}k_{+4} + k_{+3}k_{+4}k_{+5})[S_1][S_2] + k_{+1}k_{+4}(k_{-3} + k_{+5})[S_1]^2 + k_{+2}k_{+3}(k_{-4} + k_{+5})[S_2]^2 + k_{+4}k_{-5}(k_{-1} + k_{-3})[S_1][P] + k_{+3}k_{-5}(k_{-2} + k_{-4})[S_2][P] + k_{+1}k_{+3}k_{+4}[S_1]^2[S_2] + k_{+2}k_{+3}k_{+4}[S_1][S_2]^2 + k_{+3}k_{+4}k_{-5}[S_1][S_2][P]$

Substance	Max	Min	Remarks
Substrate	2	2	
Product	1	1	
Catalyst	1	1	

Parameter	Type	Unit	Description
k_1	Float		
k_{-1}	Float		
k_2	Float		
k_{-2}	Float		
k_3	Float		
k_{-3}	Float		
k_4	Float		
k_{-4}	Float		
k_5	Float		
k_{-5}	Float		

Notes

15 RandomUniBiReactor

Classname	RandomUniBiReactor
Base Class	FluxReactor
Brief Description	Random Uni Bi reaction system

Version				Date
E-CELL	ecs-v09	Reactor	0.1	30/6/1999

Author	Masayuki Okayama
E-mail	t98204mo@sfc.keio.ac.jp

Description
A reactor class for a random bireactant system in the Bi Uni direction.

Equation

$$v = \frac{M(P)\,[E]}{Den}$$

$M(P) = k_{+1}k_{+4}k_{+5}(k_{+2}+k_{+3})[S_1] + k_{+1}k_{+2}k_{+4}k_{-3}[S_1][P_1] + k_{-1}(-k_{-2}k_{-4}k_{+5} - k_{+4}k_{-3}k_{-5})[P_1][P_2] + k_{+1}k_{-2}k_{+3}k_{+5}[S_1][P_2] - k_{-1}k_{-2}k_{-4}k_{-3}[P_1]^2[P_2] - k_{-1}k_{-2}k_{-3}k_{-5}[P_1][P_2]^2$
$Den = k_{+4}k_{+5}(k_{-1}+k_{+2}+k_{+3}) + k_{+1}(k_{+2}k_{+5}+k_{+4}k_{+5}+k_{+4}k_{+3})[S_1] + (k_{-1}k_{-2}k_{+5}+k_{-2}k_{+3}k_{+5}+k_{-1}k_{+4}k_{-5}+k_{+2}k_{+4}k_{-5}+k_{+4}k_{+3}k_{-5})[P_2] + (k_{-1}k_{+4}k_{-3}+k_{+2}k_{+4}k_{-3}+k_{-1}k_{-4}k_{+5}+k_{+2}k_{-4}k_{+5}+k_{-4}k_{+3}k_{+5})[P_1] + k_{+1}k_{-3}(k_{+2}+k_{+4})[S_1][P_1] + k_{+1}k_{-2}(k_{+5}+k_{+3})[S_1][P_2] + (k_{-1}k_{-2}k_{-3}+k_{-2}k_{-4}k_{+5}+k_{-2}k_{-4}k_{+3}+k_{+2}k_{-3}k_{-5}+k_{+4}k_{-3}k_{-5})[P_1][P_2] + k_{-4}k_{-3}(k_{-1}+k_{+2})[P_1]^2 + k_{-2}k_{-5}(k_{-1}+k_{+3})[P_2]^2 + k_{+1}k_{-2}k_{-3}[S_1][P_1][P_2] + k_{-2}k_{-4}k_{-3}[P_1]^2[P_2] + k_{-2}k_{-3}k_{-5}[P_1][P_2]^2$

Substance	Max	Min	Remarks
Substrate	1	1	
Product	2	2	
Catalyst	1	1	

Parameter	Type	Unit	Description
k_1	Float		
k_{-1}	Float		
k_2	Float		
k_{-2}	Float		
k_4	Float		
k_{-4}	Float		
k_3	Float		
k_{-3}	Float		
k_5	Float		
k_{-5}	Float		

Notes

16 RapidEquilibriumPReactor

Classname	RapidEquilibriumPReactor
Base Class	Reactor
Brief Description	Binding reaction which rapidlly reaches equilibrium

Version				Date
E-CELL	ecs-1.0	Reactor	0.1	2000 2/2

Author	Kenta Hashimoto
E-mail	kem@sfc.keio.ac.jp

Description
A reactor class for binding reactions which rapidly (within a step) reaches a state of equilibrium. This reactor calculates velocity according to the equilibrium constant inputted by the user. In case that two substrates are already at a state of equilibrium, velocity is set to zero.

Equation
$$k_{eq} \prod([S_k] - v) = \prod([P_k] + v)$$

Substance	Max	Min	Remarks
Substrate	inf	1	
Product	inf	1	

Parameter	Type	Unit	Description
Keq	Float	$M^{(numberofProduct)-(numberofSubstrate)}$	Equilibrium constant

Notes
"v" is velocity.

17 RapidEquilibriumReactor

Classname	RapidEquilibriumReactor
Base Class	Reactor
Brief Description	Binding reaction which rapidlly reaches equilibrium

Version				Date
E-CELL	ecs-v08	Reactor	0.1	1999 2/22

Author	Kenta Hashimoto
E-mail	kem@sfc.keio.ac.jp

Description
A reactor class for binding reactions which rapidly (within a step) reaches a state of equilibrium. This reactor calculates velocity according to the equilibrium constant inputted by the user. In case that two substrates are already at a state of equilibrium, velocity is set to zero.

Equation
$$k_{eq}\prod([S_k]-v)=\prod([P_k]+v)$$

Substance	Max	Min	Remarks
Substrate	inf	1	
Product	inf	1	

Parameter	Type	Unit	Description
Keq	Float	$M^{(numberofProduct)-(numberofSubstrate)}$	Equilibrium constant

Notes
"v" is velosity.

18 ZeroReactor

Classname	ZeroReactor
Base Class	FluxReactor
Brief Description	Zero order reaction

Version				Date
E-CELL	ecs-v09	Reactor	0.1	29/6/1999

Author	Kouichi Takahashi
E-mail	shafi@sfc.keio.ac.jp

Description
A reactor class for zero order reaction of which flux rate is a constant. Velocity is independent of concentration of molecular species.

Equation
$v = Rate$

Substance	Max	Min	Remarks
Substrate	Inf	1	
Product	Inf	1	
Catalyst	0	0	
Effector	0	0	

Parameter	Type	Unit	Description
Rate	Float	Molecules/Second	Rate

Notes