SBML Model Report

Model name: "Tyson2003_Substrate_Depletion_Osc"

May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by Lukas Endler[1] at February tenth 2011 at 3:49 a. m. and last time modified at April sixth 2014 at 8:01 p. m. Table 1 shows an overview of the quantities of all components of this model.

Table 1: Number of components in this model, which are described in the following sections.

Element	Quantity	Element	Quantity
compartment types	0	compartments	1
species types	0	species	5
events	0	constraints	0
reactions	5	function definitions	1
global parameters	11	unit definitions	6
rules	4	initial assignments	0

Model Notes

This is an SBML implementation the model of the substrate depletion oscillator (figure 2c) described in the article:
Sniffers, buzzers, toggles and blinkers: dynamics of regulatory and signaling pathways in the cell.
Tyson JJ, Chen KC, Novak B. Curr Opin Cell Biol. 2003 Apr;15(2):221-31. PubmedID:12648679;

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DOI:10.1016/S0955-0674(03)00017-6;

Abstract:
The physiological responses of cells to external and internal stimuli are governed by genes and proteins interacting in complex networks whose dynamical properties are impossible to understand by intuitive reasoning alone. Recent advances by theoretical biologists have demonstrated that molecular regulatory networks can be accurately modeled in mathematical terms. These models shed light on the design principles of biological control systems and make predictions that have been verified experimentally.

2 Unit Definitions

This is an overview of nine unit definitions of which three are predefined by SBML and not mentioned in the model.

2.1 Unit `time`

Name s

Definition s

2.2 Unit `substance`

Name mole

Definition mol

2.3 Unit `per_s`

Name per_s

Definition s^{-1}

2.4 Unit `M_per_s`

Name M_per_s

Definition $mol \cdot s^{-1} \cdot l^{-1}$

2.5 Unit M

Name M

Definition $\mathrm{mol} \cdot \mathrm{l}^{-1}$

2.6 Unit per_M_per_s

Name per_M_per_s

Definition $\mathrm{mol}^{-1} \cdot \mathrm{l} \cdot \mathrm{s}^{-1}$

2.7 Unit volume

Notes Litre is the predefined SBML unit for `volume`.

Definition l

2.8 Unit area

Notes Square metre is the predefined SBML unit for `area` since SBML Level 2 Version 1.

Definition m^2

2.9 Unit length

Notes Metre is the predefined SBML unit for `length` since SBML Level 2 Version 1.

Definition m

3 Compartment

This model contains one compartment.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
env		0000290	3	1	litre	☑	

3.1 Compartment env

This is a three dimensional compartment with a constant size of one litre.

SBO:0000290 physical compartment

4 Species

This model contains five species. The boundary condition of three of these species is set to `true` so that these species' amount cannot be changed by any reaction. Section 9 provides further details and the derived rates of change of each species.

Table 3: Properties of each species.

Id	Name	Compartment	Derived Unit	Constant	Boundary Condition
R		env	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☐
X		env	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☐
S		env	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☑
Ep		env	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☑
E		env	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☑

5 Parameters

This model contains eleven global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k0_prime		0000035	0.01	s^{-1}	☑
k0		0000036	0.40	$mol^{-1} \cdot l \cdot s^{-1}$	☑
k1		0000035	1.00	s^{-1}	☑
k2		0000356	1.00	s^{-1}	☑
k3		0000186	1.00	s^{-1}	☑
J3		0000002	0.05	dimensionless	☑
k4		0000186	0.30	$mol \cdot s^{-1} \cdot l^{-1}$	☑
J4		0000002	0.05	dimensionless	☑
Et		0000196	1.00	$mol \cdot l^{-1}$	☑
Km3		0000027	0.00	$mol \cdot l^{-1}$	☐
Km4		0000027	0.00	$mol \cdot l^{-1}$	☐

6 Function definition

This is an overview of one function definition.

6.1 Function definition goldbeter_koshland

Arguments v1, v2, J1, J2

Mathematical Expression

$$\frac{2 \cdot v1 \cdot J2}{v2 - v1 + J1 \cdot v2 + J2 \cdot v1 + \left((v2 - v1 + J1 \cdot v2 + J2 \cdot v1)^2 - 4 \cdot (v2 - v1) \cdot v1 \cdot J2\right)^{\frac{1}{2}}} \tag{1}$$

7 Rules

This is an overview of four rules.

7.1 Rule Km3

Rule Km3 is an assignment rule for parameter Km3:

$$Km3 = J3 \cdot Et \tag{2}$$

Derived unit $mol \cdot l^{-1}$

7.2 Rule Km4

Rule Km4 is an assignment rule for parameter Km4:

$$\mathrm{Km4} = \mathrm{J4} \cdot \mathrm{Et} \tag{3}$$

Derived unit $\mathrm{mol} \cdot \mathrm{l}^{-1}$

7.3 Rule Ep

Rule Ep is an assignment rule for species Ep:

$$\mathrm{Ep} = \mathrm{goldbeter\_koshland}\left(\mathrm{k3} \cdot [\mathrm{R}], \mathrm{k4}, \mathrm{J3}, \mathrm{J4}\right) \cdot \mathrm{Et} \tag{4}$$

7.4 Rule E

Rule E is an assignment rule for species E:

$$\mathrm{E} = \mathrm{Et} - [\mathrm{Ep}] \tag{5}$$

Derived unit $\mathrm{mol} \cdot \mathrm{l}^{-1}$

8 Reactions

This model contains five reactions. All reactions are listed in the following table and are subsequently described in detail. If a reaction is affected by a modifier, the identifier of this species is written above the reaction arrow.

Table 5: Overview of all reactions

№	Id	Name	Reaction Equation	SBO
1	r0		$X \xrightarrow{Ep} R$	0000182
2	r1		$\emptyset \xrightarrow{S} X$	0000176
3	r2		$R \longrightarrow \emptyset$	0000179
4	r3		$E \xrightarrow{R} Ep$	0000216
5	r4		$Ep \longrightarrow E$	0000330

8.1 Reaction r0

This is an irreversible reaction of one reactant forming one product influenced by one modifier.

SBO:0000182 conversion

Reaction equation

$$\mathrm{X} \xrightarrow{\mathrm{Ep}} \mathrm{R} \tag{6}$$

Reactant

Table 6: Properties of each reactant.

Id	Name	SBO
X		

Modifier

Table 7: Properties of each modifier.

Id	Name	SBO
Ep		0000462

Product

Table 8: Properties of each product.

Id	Name	SBO
R		

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{mol}$

$$v_1 = \mathrm{vol}\,(\mathrm{env}) \cdot (\mathrm{k0\_prime} + \mathrm{k0} \cdot [\mathrm{Ep}]) \cdot [\mathrm{X}] \tag{7}$$

8.2 Reaction r1

This is an irreversible reaction of no reactant forming one product influenced by one modifier.

SBO:0000176 biochemical reaction

Reaction equation

$$\emptyset \xrightarrow{S} X \tag{8}$$

Modifier

Table 9: Properties of each modifier.

Id	Name	SBO
S		0000461

Product

Table 10: Properties of each product.

Id	Name	SBO
X		

Kinetic Law

SBO:0000049 mass action rate law for first order irreversible reactions, continuous scheme

Derived unit $s^{-1} \cdot mol$

$$v_2 = \mathrm{vol}(\mathrm{env}) \cdot k1 \cdot [S] \tag{9}$$

8.3 Reaction r2

This is an irreversible reaction of one reactant forming no product.

SBO:0000179 degradation

Reaction equation

$$R \longrightarrow \emptyset \tag{10}$$

Reactant

Table 11: Properties of each reactant.

Id	Name	SBO
R		

Kinetic Law

SBO:0000049 mass action rate law for first order irreversible reactions, continuous scheme

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{mol}$

$$v_3 = \mathrm{vol}\,(\mathrm{env}) \cdot \mathrm{k2} \cdot [\mathrm{R}] \tag{11}$$

8.4 Reaction r3

This is an irreversible reaction of one reactant forming one product influenced by one modifier.

SBO:0000216 phosphorylation

Reaction equation

$$\mathrm{E} \xrightarrow{\mathrm{R}} \mathrm{Ep} \tag{12}$$

Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
E		

Modifier

Table 13: Properties of each modifier.

Id	Name	SBO
R		0000461

Product

Table 14: Properties of each product.

Id	Name	SBO
Ep		

Kinetic Law

SBO:0000430 enzymatic rate law for modulated unireactant enzymes

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{mol}$

$$v_4 = \frac{\mathrm{vol}\,(\mathrm{env}) \cdot \mathrm{k3} \cdot [\mathrm{R}] \cdot [\mathrm{E}]}{\mathrm{Km3} + [\mathrm{E}]} \tag{13}$$

8.5 Reaction r4

This is an irreversible reaction of one reactant forming one product.

SBO:0000330 dephosphorylation

Reaction equation

$$\mathrm{Ep} \longrightarrow \mathrm{E} \tag{14}$$

Reactant

Table 15: Properties of each reactant.

Id	Name	SBO
Ep		

Product

Table 16: Properties of each product.

Id	Name	SBO
E		

Kinetic Law

SBO:0000199 normalised enzymatic rate law for unireactant enzymes

Derived unit $\mathrm{mol} \cdot \mathrm{s}^{-1}$

$$v_5 = \frac{\mathrm{vol}\,(\mathrm{env}) \cdot \mathrm{k4} \cdot [\mathrm{Ep}]}{\mathrm{Km4} + [\mathrm{Ep}]} \tag{15}$$

9 Derived Rate Equations

When interpreted as an ordinary differential equation framework, this model implies the following set of equations for the rates of change of each species.

9.1 Species R

SBO:0000285 material entity of unspecified nature

Initial concentration $0\ \mathrm{mol} \cdot \mathrm{l}^{-1}$

This species takes part in three reactions (as a reactant in r2 and as a product in r0 and as a modifier in r3).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{R} = v_1 - v_3 \tag{16}$$

9.2 Species X

SBO:0000285 material entity of unspecified nature

Initial concentration $0\ \mathrm{mol} \cdot \mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in r0 and as a product in r1).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{X} = v_2 - v_1 \tag{17}$$

9.3 Species S

SBO:0000285 material entity of unspecified nature

Initial concentration $0\ \mathrm{mol} \cdot \mathrm{l}^{-1}$

This species takes part in one reaction (as a modifier in r1), which does not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{S} = 0 \tag{18}$$

9.4 Species Ep

SBO:0000252 polypeptide chain

Involved in rule Ep

This species takes part in three reactions (as a reactant in r4 and as a product in r3 and as a modifier in r0). Not these but one rule determines the species' quantity because this species is on the boundary of the reaction system.

9.5 Species E

SBO:0000252 polypeptide chain

Involved in rule E

This species takes part in two reactions (as a reactant in r3 and as a product in r4). Not these but one rule determines the species' quantity because this species is on the boundary of the reaction system.

A Glossary of Systems Biology Ontology Terms

SBO:0000002 quantitative systems description parameter: A numerical value that defines certain characteristics of systems or system functions. It may be part of a calculation, but its value is not determined by the form of the equation itself, and may be arbitrarily assigned

SBO:0000027 Michaelis constant: Substrate concentration at which the velocity of reaction is half its maximum. Michaelis constant is an experimental parameter. According to the underlying molecular mechanism it can be interpreted differently in terms of microscopic constants

SBO:0000035 forward unimolecular rate constant, continuous case: Numerical parameter that quantifies the forward velocity of a chemical reaction involving only one reactant. This parameter encompasses all the contributions to the velocity except the quantity of the reactant. It is to be used in a reaction modelled using a continuous framework

SBO:0000036 forward bimolecular rate constant, continuous case: Numerical parameter that quantifies the forward velocity of a chemical reaction involving two reactants. This parameter encompasses all the contributions to the velocity except the quantity of the reactants. It is to be used in a reaction modelled using a continuous framework

SBO:0000049 mass action rate law for first order irreversible reactions, continuous scheme: Reaction scheme where the products are created from the reactants and the change of a product quantity is proportional to the product of reactant activities. The reaction scheme does not include any reverse process that creates the reactants from the products. The change of a product quantity is proportional to the quantity of one reactant. It is to be used in a reaction modelled using a continuous framework.

SBO:0000176 biochemical reaction: An event involving one or more chemical entities that modifies the electrochemical structure of at least one of the participants.

SBO:0000179 degradation: Complete disappearance of a physical entity

SBO:0000182 conversion: Biochemical reaction that results in the modification of some covalent bonds

SBO:0000186 maximal velocity: Limiting maximal velocity of an enzymatic reaction, reached when the substrate is in large excess and all the enzyme is complexed.

SBO:0000196 concentration of an entity pool: The amount of an entity per unit of volume.

SBO:0000199 normalised enzymatic rate law for unireactant enzymes: Kinetics of enzymes that react only with one substance, their substrate. The total enzyme concentration is considered to be equal to 1, therefore the maximal velocity equals the catalytic constant.

SBO:0000216 phosphorylation: Addition of a phosphate group (-H2PO4) to a chemical entity

SBO:0000252 polypeptide chain: Naturally occurring macromolecule formed by the repetition of amino-acid residues linked by peptidic bonds. A polypeptide chain is synthesized by the ribosome. CHEBI:1654

SBO:0000285 material entity of unspecified nature: Material entity whose nature is unknown or irrelevant

SBO:0000290 physical compartment: Specific location of space, that can be bounded or not. A physical compartment can have 1, 2 or 3 dimensions

SBO:0000330 dephosphorylation: Removal of a phosphate group (-H2PO4) from a chemical entity.

SBO:0000356 decay constant: Kinetic constant characterising a mono-exponential decay. It is the inverse of the mean lifetime of the continuant being decayed. Its unit is“per tim”.

SBO:0000430 enzymatic rate law for modulated unireactant enzymes: Kinetics of enzymes that react with one substance, and whose activity may be positively or negatively modulated

SBO:0000461 essential activator: A substance that is absolutely required for occurrence and stimulation of a reaction

SBO:0000462 non-essential activator: An activator which is not necessary for an enzymatic reaction, but whose presence will further increase enzymatic activity.

SBML2LaTeX was developed by Andreas Dräger[a], Hannes Planatscher[a], Dieudonné M Wouamba[a], Adrian Schröder[a], Michael Hucka[b], Lukas Endler[c], Martin Golebiewski[d] and Andreas Zell[a]. Please see http://www.ra.cs.uni-tuebingen.de/software/SBML2LaTeX for more information.

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