SBML Model Report

Model name: "Piedrafita2010_MR_System"

May 5, 2016

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by Lukas Endler[1] at August nineth 2010 at 4:31 p. m. and last time modified at April fourth 2014 at 5:44 p. m. Table 1 provides 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	11
events	0	constraints	0
reactions	11	function definitions	0
global parameters	19	unit definitions	5
rules	2	initial assignments	0

Model Notes

This is the self maintaining metabolism model described in the article:
A Simple Self-Maintaining Metabolic System: Robustness, Autocatalysis, Bistability.
Piedrafita G, Montero F, Morn F, Crdenas ML, Cornish-Bowden A, PLoS Computational Biology 2010, 6(8):e1000872. doi:10.1371/journal.pcbi.1000872
Abstract:
A living organism must not only organize itself from within; it must also maintain its organization in the face of changes in its environment and degradation of its components. We show

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here that a simple (M,R)-system consisting of three interlocking catalytic cycles, with every catalyst produced by the system itself, can both establish a non-trivial steady state and maintain this despite continuous loss of the catalysts by irreversible degradation. As long as at least one catalyst is present at a sufficient concentration in the initial state, the others can be produced and maintained. The system shows bistability, because if the amount of catalyst in the initial state is insufficient to reach the non-trivial steady state the system collapses to a trivial steady state in which all fluxes are zero. It is also robust, because if one catalyst is catastrophically lost when the system is in steady state it can recreate the same state. There are three elementary flux modes, but none of them is an enzyme-maintaining mode, the entire network being necessary to maintain the two catalysts

As this is a theoretical model and no units are given in the article, the standard units (mol, seconds and litre) are used for the parameters. k8 and k11 are set equal to k4.

Originally created by libAntimony v1.4 (using libSBML 3.4.1)

2 Unit Definitions

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

2.1 Unit `substance`

Name mole

Definition mol

2.2 Unit `time`

Name sec

Definition s

2.3 Unit `volume`

Name litre

Definition l

2.4 Unit `per_time`

Name per_time

Definition s^{-1}

2.5 Unit per_time_per_M

Name per_time_per_M

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

2.6 Unit area

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

Definition m^2

2.7 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	environment	0000290	3	1	litre	☑	

3.1 Compartment env

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

Name environment

SBO:0000290 physical compartment

4 Species

This model contains eleven 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 8 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
S		env	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	☑
U		env	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	☑
T		env	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	☑
STU		env	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
STUS		env	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
STUST		env	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
STUSU		env	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
SU		env	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
ST		env	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
SUST		env	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
SUSTU		env	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟

5 Parameters

This model contains 19 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1		0000339	10.00	$mol^{-1} \cdot s^{-1} \cdot l$	☑
k1r		0000038	10.00	s^{-1}	☑
k2		0000339	10.00	$mol^{-1} \cdot s^{-1} \cdot l$	☑
k2r		0000038	10.00	s^{-1}	☑
k3		0000035	2.00	s^{-1}	☑
k3r		0000039	1.00	$mol^{-1} \cdot s^{-1} \cdot l$	☑
k4		0000035	0.30	s^{-1}	☑
k5		0000339	1.00	$mol^{-1} \cdot s^{-1} \cdot l$	☑
k5r		0000038	1.00	s^{-1}	☑
k6		0000339	1.00	$mol^{-1} \cdot s^{-1} \cdot l$	☑
k6r		0000038	1.00	s^{-1}	☑
k7		0000035	0.10	s^{-1}	☑
k7r		0000039	0.10	$mol^{-1} \cdot s^{-1} \cdot l$	☑
k8		0000035	0.00	s^{-1}	⊟
k9		0000339	0.10	$mol^{-1} \cdot s^{-1} \cdot l$	☑
k9r		0000038	0.05	s^{-1}	☑
k10		0000035	0.05	s^{-1}	☑
k10r		0000039	0.05	$mol^{-1} \cdot s^{-1} \cdot l$	☑
k11		0000035	0.00	s^{-1}	⊟

6 Rules

This is an overview of two rules.

6.1 Rule k8

Rule k8 is an assignment rule for parameter k8:

$$k8 = k4 \tag{1}$$

Derived unit s^{-1}

6.2 Rule k11

Rule k11 is an assignment rule for parameter k11:

$$k11 = k4 \tag{2}$$

Derived unit s^{-1}

7 Reactions

This model contains eleven 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	`reaction1`		$S + STU \rightleftharpoons STUS$	0000210
2	`reaction2`		$T + STUS \rightleftharpoons STUST$	0000210
3	`reaction3`		$STUST \rightleftharpoons ST + STU$	0000178
4	`reaction4`		$STU \longrightarrow \emptyset$	0000179
5	`reaction5`		$SU + ST \rightleftharpoons SUST$	0000210
6	`reaction6`		$U + SUST \rightleftharpoons SUSTU$	0000210
7	`reaction7`		$SUSTU \rightleftharpoons STU + SU$	0000178
8	`reaction8`		$SU \longrightarrow \emptyset$	0000179
9	`reaction9`		$U + STUS \rightleftharpoons STUSU$	0000210
10	`reaction10`		$STUSU \rightleftharpoons STU + SU$	0000178
11	`reaction11`		$ST \longrightarrow \emptyset$	0000179

7.1 Reaction `reaction1`

This is a reversible reaction of two reactants forming one product.

SBO:0000210 addition of a chemical group

Reaction equation

$$\mathrm{S} + \mathrm{STU} \rightleftharpoons \mathrm{STUS} \tag{3}$$

Reactants

Table 6: Properties of each reactant.

Id	Name	SBO
S		
STU		

Product

Table 7: Properties of each product.

Id	Name	SBO
STUS		

Kinetic Law

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

$$v_1 = \mathrm{vol}\,(\mathrm{env}) \cdot (\mathrm{k1} \cdot [\mathrm{S}] \cdot [\mathrm{STU}] - \mathrm{k1r} \cdot [\mathrm{STUS}]) \tag{4}$$

7.2 Reaction `reaction2`

This is a reversible reaction of two reactants forming one product.

SBO:0000210 addition of a chemical group

Reaction equation

$$\mathrm{T} + \mathrm{STUS} \rightleftharpoons \mathrm{STUST} \tag{5}$$

Reactants

Table 8: Properties of each reactant.

Id	Name	SBO
T		
STUS		

Product

Table 9: Properties of each product.

Id	Name	SBO
STUST		

Kinetic Law

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

$$v_2 = \mathrm{vol}\,(\mathrm{env}) \cdot (\mathrm{k2} \cdot [\mathrm{T}] \cdot [\mathrm{STUS}] - \mathrm{k2r} \cdot [\mathrm{STUST}]) \tag{6}$$

7.3 Reaction `reaction3`

This is a reversible reaction of one reactant forming two products.

SBO:0000178 cleavage

Reaction equation

$$\mathrm{STUST} \rightleftharpoons \mathrm{ST} + \mathrm{STU} \tag{7}$$

Reactant

Table 10: Properties of each reactant.

Id	Name	SBO
STUST		

Products

Table 11: Properties of each product.

Id	Name	SBO
ST		

Id	Name	SBO
STU		

Kinetic Law

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

$$v_3 = \mathrm{vol}(\mathrm{env}) \cdot (\mathrm{k3} \cdot [\mathrm{STUST}] - \mathrm{k3r} \cdot [\mathrm{ST}] \cdot [\mathrm{STU}]) \tag{8}$$

7.4 Reaction `reaction4`

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

SBO:0000179 degradation

Reaction equation

$$\mathrm{STU} \longrightarrow \emptyset \tag{9}$$

Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
STU		

Kinetic Law

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

$$v_4 = \mathrm{vol}(\mathrm{env}) \cdot \mathrm{k4} \cdot [\mathrm{STU}] \tag{10}$$

7.5 Reaction `reaction5`

This is a reversible reaction of two reactants forming one product.

SBO:0000210 addition of a chemical group

Reaction equation

$$\mathrm{SU} + \mathrm{ST} \rightleftharpoons \mathrm{SUST} \tag{11}$$

Reactants

Table 13: Properties of each reactant.

Id	Name	SBO
SU		
ST		

Product

Table 14: Properties of each product.

Id	Name	SBO
SUST		

Kinetic Law

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

$$v_5 = \mathrm{vol}\,(\mathrm{env}) \cdot (\mathrm{k5} \cdot [\mathrm{ST}] \cdot [\mathrm{SU}] - \mathrm{k5r} \cdot [\mathrm{SUST}]) \tag{12}$$

7.6 Reaction `reaction6`

This is a reversible reaction of two reactants forming one product.

SBO:0000210 addition of a chemical group

Reaction equation

$$\mathrm{U} + \mathrm{SUST} \rightleftharpoons \mathrm{SUSTU} \tag{13}$$

Reactants

Table 15: Properties of each reactant.

Id	Name	SBO
U		
SUST		

Product

Table 16: Properties of each product.

Id	Name	SBO
SUSTU		

Kinetic Law

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

$$v_6 = \mathrm{vol}(\mathrm{env}) \cdot (\mathrm{k6} \cdot [\mathrm{U}] \cdot [\mathrm{SUST}] - \mathrm{k6r} \cdot [\mathrm{SUSTU}]) \tag{14}$$

7.7 Reaction `reaction7`

This is a reversible reaction of one reactant forming two products.

SBO:0000178 cleavage

Reaction equation

$$\mathrm{SUSTU} \rightleftharpoons \mathrm{STU} + \mathrm{SU} \tag{15}$$

Reactant

Table 17: Properties of each reactant.

Id	Name	SBO
SUSTU		

Products

Table 18: Properties of each product.

Id	Name	SBO
STU		
SU		

Kinetic Law

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

$$v_7 = \mathrm{vol}(\mathrm{env}) \cdot (\mathrm{k7} \cdot [\mathrm{SUSTU}] - \mathrm{k7r} \cdot [\mathrm{STU}] \cdot [\mathrm{SU}]) \tag{16}$$

7.8 Reaction `reaction8`

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

SBO:0000179 degradation

Reaction equation

$$\mathrm{SU} \longrightarrow \emptyset \tag{17}$$

Reactant

Table 19: Properties of each reactant.

Id	Name	SBO
SU		

Kinetic Law

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

$$v_8 = \mathrm{vol}\,(\mathrm{env}) \cdot \mathrm{k8} \cdot [\mathrm{SU}] \tag{18}$$

7.9 Reaction `reaction9`

This is a reversible reaction of two reactants forming one product.

SBO:0000210 addition of a chemical group

Reaction equation

$$\mathrm{U} + \mathrm{STUS} \rightleftharpoons \mathrm{STUSU} \tag{19}$$

Reactants

Table 20: Properties of each reactant.

Id	Name	SBO
U		
STUS		

Product

Table 21: Properties of each product.

Id	Name	SBO
STUSU		

Kinetic Law

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

$$v_9 = \mathrm{vol}(\mathrm{env}) \cdot (\mathrm{k9} \cdot [\mathrm{U}] \cdot [\mathrm{STUS}] - \mathrm{k9r} \cdot [\mathrm{STUSU}]) \tag{20}$$

7.10 Reaction `reaction10`

This is a reversible reaction of one reactant forming two products.

SBO:0000178 cleavage

Reaction equation

$$\mathrm{STUSU} \rightleftharpoons \mathrm{STU} + \mathrm{SU} \tag{21}$$

Reactant

Table 22: Properties of each reactant.

Id	Name	SBO
STUSU		

Products

Table 23: Properties of each product.

Id	Name	SBO
STU		
SU		

Kinetic Law

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

$$v_{10} = \mathrm{vol}(\mathrm{env}) \cdot (\mathrm{k10} \cdot [\mathrm{STUSU}] - \mathrm{k10r} \cdot [\mathrm{STU}] \cdot [\mathrm{SU}]) \tag{22}$$

7.11 Reaction reaction11

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

SBO:0000179 degradation

Reaction equation

$$\mathrm{ST} \longrightarrow \emptyset \tag{23}$$

Reactant

Table 24: Properties of each reactant.

Id	Name	SBO
ST		

Kinetic Law

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

$$v_{11} = \mathrm{vol}\,(\mathrm{env}) \cdot \mathrm{k11} \cdot [\mathrm{ST}] \tag{24}$$

8 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.

8.1 Species S

SBO:0000240 material entity

Initial concentration $4\ \mathrm{mol} \cdot \mathrm{l}^{-1}$

This species takes part in one reaction (as a reactant in reaction1), which does not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{S} = 0 \tag{25}$$

8.2 Species U

SBO:0000240 material entity

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

This species takes part in two reactions (as a reactant in reaction6, reaction9), which do not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{U} = 0 \tag{26}$$

8.3 Species T

SBO:0000240 material entity

Initial concentration $2\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in one reaction (as a reactant in reaction2), which does not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{T} = 0 \tag{27}$$

8.4 Species STU

SBO:0000240 material entity

Initial concentration $5\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in five reactions (as a reactant in reaction1, reaction4 and as a product in reaction3, reaction7, reaction10).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{STU} = v_3 + v_7 + v_{10} - v_1 - v_4 \tag{28}$$

8.5 Species STUS

SBO:0000240 material entity

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

This species takes part in three reactions (as a reactant in reaction2, reaction9 and as a product in reaction1).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{STUS} = v_1 - v_2 - v_9 \tag{29}$$

8.6 Species STUST

SBO:0000240 material entity

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

This species takes part in two reactions (as a reactant in reaction3 and as a product in reaction2).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{STUST} = v_2 - v_3 \tag{30}$$

8.7 Species STUSU

SBO:0000240 material entity

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

This species takes part in two reactions (as a reactant in reaction10 and as a product in reaction9).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{STUSU} = v_9 - v_{10} \tag{31}$$

8.8 Species SU

SBO:0000240 material entity

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

This species takes part in four reactions (as a reactant in reaction5, reaction8 and as a product in reaction7, reaction10).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{SU} = v_7 + v_{10} - v_5 - v_8 \tag{32}$$

8.9 Species ST

SBO:0000240 material entity

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

This species takes part in three reactions (as a reactant in reaction5, reaction11 and as a product in reaction3).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ST} = v_3 - v_5 - v_{11} \tag{33}$$

8.10 Species SUST

SBO:0000240 material entity

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

This species takes part in two reactions (as a reactant in reaction6 and as a product in reaction5).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{SUST} = v_5 - v_6 \tag{34}$$

8.11 Species SUSTU

SBO:0000240 material entity

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

This species takes part in two reactions (as a reactant in reaction7 and as a product in reaction6).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{SUSTU} = v_6 - v_7 \tag{35}$$

A Glossary of Systems Biology Ontology Terms

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:0000038 **reverse unimolecular rate constant, continuous case:** Numerical parameter that quantifies the reverse velocity of a chemical reaction involving only one product. This parameter encompasses all the contributions to the velocity except the quantity of the product. It is to be used in a reaction modelled using a continuous framework

SBO:0000039 **reverse bimolecular rate constant, continuous case:** Numerical parameter that quantifies the reverse velocity of a chemical reaction involving only one product. This parameter encompasses all the contributions to the velocity except the quantity of the product. It is to be used in a reaction modelled using a continuous framework

SBO:0000178 **cleavage:** Rupture of a covalent bond resulting in the conversion of one physical entity into several physical entities

SBO:0000179 **degradation:** Complete disappearance of a physical entity

SBO:0000210 **addition of a chemical group:** Covalent reaction that results in the addition of a chemical group on a molecule

SBO:0000240 **material entity:** A real thing that is defined by its physico-chemical structure.

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:0000339 **bimolecular association rate constant:** Rate with which two components associate into a complex

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