SBML Model Report

Model name: "Decroly1982_Enzymatic_Oscillator"

May 5, 2016

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by Kieran Smallbone[1] at August eleventh 2010 at 1:53 p. m. and last time modified at February 25th 2015 at 11:36 a. 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	3
events	0	constraints	0
reactions	4	function definitions	0
global parameters	0	unit definitions	3
rules	0	initial assignments	0

Model Notes

This is the scaled model described in the article:
Birhythmicity, chaos, and other patterns of temporal self-organization in a multiply regulated biochemical system
Olivier Decroly, Albert Goldbeter, *Proc Natl Acad Sci USA* 1982 79:6917-6921; PMID:6960354;

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Abstract:
We analyze on a model biochemical system the effect of a coupling between two instability-generating mechanisms. The system considered is that of two allosteric enzymes coupled in series and activated by their respective products. In addition to simple periodic oscillations, the system can exhibit a variety of new modes of dynamic behavior; coexistence between two stable periodic regimes (birhythmicity), random oscillations (chaos), and coexistence of a stable periodic regime with a stable steady state (hard excitation) or with chaos. The relationship between these patterns of temporal self-organization is analyzed as a function of the control parameters of the model. Chaos and birhythmicity appear to be rare events in comparison with simple periodic behavior. We discuss the relevance of these results with respect to the regularity of most biological rhythms.

The parameters q1 = 50 and q2 = 0.02 are explicitely included as the stoichiometric coefficients of beta and gamma in the reactions r2 and r3, respectively. Parameter values and initial conditions [ks=1.99/sec, alpha(0)=29.19988, beta(0)=188.8, gamma(0)=0.3367] are for the chaotic regime presented in the upper-curve of Figure 3b.

2 Unit Definitions

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

2.1 Unit `substance`

Definition dimensionless

2.2 Unit `volume`

Definition dimensionless

2.3 Unit `per_sec`

Name per sec

Definition s^{-1}

2.4 Unit `area`

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

Definition m^2

2.5 Unit `length`

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

Definition m

2.6 Unit `time`

Notes Second is the predefined SBML unit for `time`.

Definition s

3 Compartment

This model contains one compartment.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
`cell`	cell		3	1	dimensionless	☑	

3.1 Compartment `cell`

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

Name cell

4 Species

This model contains three species. Section 6 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
`alpha`	alpha	`cell`	dimensionless · dimensionless^{-1}	⊟	⊟
`beta`	beta	`cell`	dimensionless · dimensionless^{-1}	⊟	⊟
`gamma`	gamma	`cell`	dimensionless · dimensionless^{-1}	⊟	⊟

5 Reactions

This model contains four 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 4: Overview of all reactions

№	Id	Name	Reaction Equation	SBO
1	r1		$\emptyset \longrightarrow$ alpha	0000176
2	r2		alpha $\longrightarrow 50$ beta	0000176
3	r3		beta $\longrightarrow 0 \cdot 02$ gamma	0000176
4	r4		gamma $\longrightarrow \emptyset$	0000179

5.1 Reaction r1

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

SBO:0000176 biochemical reaction

Reaction equation

$$\emptyset \longrightarrow \text{alpha} \tag{1}$$

Product

Table 5: Properties of each product.

Id	Name	SBO
alpha	alpha	

Kinetic Law

Derived unit s^{-1}

$$v_1 = \text{v\_Km1} \tag{2}$$

Table 6: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
v_Km1		0000048	0.45	s^{-1}	☑

5.2 Reaction r2

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

SBO:0000176 biochemical reaction

Reaction equation

$$\text{alpha} \longrightarrow 50\,\text{beta} \tag{3}$$

Reactant

Table 7: Properties of each reactant.

Id	Name	SBO
alpha	alpha	

Product

Table 8: Properties of each product.

Id	Name	SBO
beta	beta	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \frac{\text{sigma1} \cdot [\text{alpha}] \cdot (1 + [\text{alpha}]) \cdot (1 + [\text{beta}])^2}{\text{L1} + (1 + [\text{alpha}])^2 \cdot (1 + [\text{beta}])^2} \tag{4}$$

Table 9: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
L1			$5 \cdot 10^8$	dimensionless	☑
sigma1		0000186	10.000	s^{-1}	☑

5.3 Reaction r3

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

SBO:0000176 biochemical reaction

Reaction equation

$$\text{beta} \longrightarrow 0{\cdot}02\,\text{gamma} \tag{5}$$

Reactant

Table 10: Properties of each reactant.

Id	Name	SBO
beta	beta	

Product

Table 11: Properties of each product.

Id	Name	SBO
gamma	gamma	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \frac{\text{sigma2} \cdot [\text{beta}] \cdot (1 + \text{d} \cdot [\text{beta}]) \cdot (1 + [\text{gamma}])^2}{\text{L2} + (1 + \text{d} \cdot [\text{beta}])^2 \cdot (1 + [\text{gamma}])^2} \tag{6}$$

Table 12: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
L2			100.0	dimensionless	☑
d			0.0	dimensionless	☑
sigma2		0000186	10.0	s^{-1}	☑

5.4 Reaction r4

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

SBO:0000179 degradation

Reaction equation

$$\text{gamma} \longrightarrow \emptyset \tag{7}$$

Reactant

Table 13: Properties of each reactant.

Id	Name	SBO
gamma	gamma	

Kinetic Law

Derived unit s^{-1}

$$v_4 = \mathrm{ks} \cdot [\mathrm{gamma}] \tag{8}$$

Table 14: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
ks		0000356	1.99	s^{-1}	☑

6 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.

Identifiers for kinetic laws highlighted in gray cannot be verified to evaluate to units of SBML `substance` per `time`. As a result, some SBML interpreters may not be able to verify the consistency of the units on quantities in the model. Please check if

- parameters without an unit definition are involved or
- volume correction is necessary because the `hasOnlySubstanceUnits` flag may be set to `false` and `spacialDimensions`> 0 for certain species.

6.1 Species `alpha`

Name alpha

SBO:0000247 simple chemical

Initial concentration 29.19988 dimensionless $\cdot$ dimensionless^{-1}

This species takes part in two reactions (as a reactant in `r2` and as a product in `r1`).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{alpha} = v_1 - v_2 \tag{9}$$

6.2 Species `beta`

Name beta

SBO:0000247 simple chemical

Initial concentration 188.8 dimensionless $\cdot$ dimensionless^{-1}

This species takes part in two reactions (as a reactant in `r3` and as a product in `r2`).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{beta} = 50\, v_2 - v_3 \tag{10}$$

6.3 Species gamma

Name gamma

SBO:0000247 simple chemical

Initial concentration $0.3367\ \text{dimensionless} \cdot \text{dimensionless}^{-1}$

This species takes part in two reactions (as a reactant in r4 and as a product in r3).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{gamma} = 0.02\ v_3 - v_4 \tag{11}$$

A Glossary of Systems Biology Ontology Terms

SBO:0000048 forward zeroth order rate constant, continuous case: Numerical parameter that quantifies the forward velocity of a chemical reaction independant of the reactant quantities. This parameter encompasses all the contributions to the velocity. 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: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:0000247 simple chemical: Simple, non-repetitive 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”.

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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