SBML Model Report

Model name: "Laub1998_SpontaneousOscillations"

May 5, 2016

1 General Overview

This is a document in SBML Level 2 Version 1 format. This model was created by Enuo He[1] at March 21st 2007 at 1:23 p. m. and last time modified at February 25th 2015 at 12:35 a. m. Table 1 gives 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	2
species types	0	species	7
events	0	constraints	0
reactions	14	function definitions	0
global parameters	14	unit definitions	2
rules	0	initial assignments	0

Model Notes

This is model according to the paper „A Molecular Network That Produces Spontaneous Oscillations in Excitalbe Cells of Dictyostelium. Figure 3 has been reproduced by Copasi 4.0.20(development) „. However four of the parameters have been changed , see details in notes.

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2 Unit Definitions

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

2.1 Unit `time`

Name min

Definition 60 s

2.2 Unit `substance`

Name micro_Mole

Definition µmol

2.3 Unit `volume`

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

Definition l

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

3 Compartments

This model contains two compartments.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
compartment_0	Extracellular		3	1	litre	☑	
compartment_1	Intracellular		3	1	litre	☑	compartment_0

3.1 Compartment compartment_0

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

Name Extracellular

3.2 Compartment compartment_1

This is a three dimensional compartment with a constant size of one litre, which is surrounded by compartment_0 (Extracellular).

Name Intracellular

4 Species

This model contains seven species. Section 7 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
species_0	Ex_cAMP	compartment_0	$\mu mol \cdot l^{-1}$	⊟	⊟
species_1	In_cAMP	compartment_1	$\mu mol \cdot l^{-1}$	⊟	⊟
species_2	PKA	compartment_1	$\mu mol \cdot l^{-1}$	⊟	⊟
species_3	REGA	compartment_1	$\mu mol \cdot l^{-1}$	⊟	⊟
species_4	ACA	compartment_1	$\mu mol \cdot l^{-1}$	⊟	⊟
species_5	CAR1	compartment_1	$\mu mol \cdot l^{-1}$	⊟	⊟
species_6	ERK2	compartment_1	$\mu mol \cdot l^{-1}$	⊟	⊟

5 Parameters

This model contains 14 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
parameter_0	k1		1.40		☑
parameter_1	k2		0.90		☑
parameter_2	k3		2.50		☑
parameter_3	k4		1.50		☑
parameter_4	k5		0.60		☑
parameter_5	k6		0.80		☑
parameter_6	k7		2.00		☑
parameter_7	k8		1.30		☑
parameter_8	k9		0.29		☑
parameter_9	k10		1.00		☑
parameter_10	k11		0.60		☑
parameter_11	k12		3.10		☑
parameter_12	k13		33.00		☑
parameter_13	k14		4.50		☑

6 Reactions

This model contains 14 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	reaction_0	k1	$\emptyset \xrightarrow{\text{species\_6}} \text{species\_4}$	
2	reaction_1	k2	$\text{species\_4} \longrightarrow \emptyset$	
3	reaction_2	k3	$\emptyset \xrightarrow{\text{species\_1}} \text{species\_2}$	
4	reaction_3	k4	$\text{species\_2} \longrightarrow \emptyset$	
5	reaction_4	k5	$\emptyset \xrightarrow{\text{species\_5}} \text{species\_6}$	
6	reaction_5	k6	$\text{species\_6} \xrightarrow{\text{species\_2}} \emptyset$	
7	reaction_6	k7	$\emptyset \longrightarrow \text{species\_3}$	
8	reaction_7	k8	$\text{species\_3} \xrightarrow{\text{species\_6}} \emptyset$	
9	reaction_8	k9	$\emptyset \xrightarrow{\text{species\_4}} \text{species\_1}$	
10	reaction_9	k10	$\text{species\_1} \xrightarrow{\text{species\_3}} \emptyset$	
11	reaction_10	k11	$\emptyset \xrightarrow{\text{species\_4}} \text{species\_0}$	
12	reaction_11	k12	$\text{species\_0} \longrightarrow \emptyset$	
13	reaction_12	k13	$\emptyset \xrightarrow{\text{species\_0}} \text{species\_5}$	
14	reaction_13	k14	$\text{species\_5} \xrightarrow{\text{species\_2}} \emptyset$	

6.1 Reaction reaction_0

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

Name k1

Reaction equation

$$\emptyset \xrightarrow{\text{species\_6}} \text{species\_4} \tag{1}$$

Modifier

Table 6: Properties of each modifier.

Id	Name	SBO
species_6	ERK2	

Product

Table 7: Properties of each product.

Id	Name	SBO
species_4	ACA	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \text{vol}(\text{compartment\_1}) \cdot \text{parameter\_0} \cdot [\text{species\_6}] \tag{2}$$

6.2 Reaction reaction_1

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

Name k2

Reaction equation

$$\text{species\_4} \longrightarrow \emptyset \tag{3}$$

Reactant

Table 8: Properties of each reactant.

Id	Name	SBO
species_4	ACA	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \mathrm{vol}\,(\mathrm{compartment\_1}) \cdot \mathrm{parameter\_1} \cdot [\mathrm{species\_4}] \tag{4}$$

6.3 Reaction reaction_2

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

Name k3

Reaction equation

$$\emptyset \xrightarrow{\mathrm{species\_1}} \mathrm{species\_2} \tag{5}$$

Modifier

Table 9: Properties of each modifier.

Id	Name	SBO
species_1	In_cAMP	

Product

Table 10: Properties of each product.

Id	Name	SBO
species_2	PKA	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \mathrm{vol}\,(\mathrm{compartment\_1}) \cdot \mathrm{parameter\_2} \cdot [\mathrm{species\_1}] \tag{6}$$

6.4 Reaction reaction_3

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

Name k4

Reaction equation

$$\text{species\_2} \longrightarrow \emptyset \tag{7}$$

Reactant

Table 11: Properties of each reactant.

Id	Name	SBO
species_2	PKA	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \text{vol}\left(\text{compartment\_1}\right) \cdot \text{parameter\_3} \cdot [\text{species\_2}] \tag{8}$$

6.5 Reaction reaction_4

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

Name k5

Reaction equation

$$\emptyset \xrightarrow{\text{species\_5}} \text{species\_6} \tag{9}$$

Modifier

Table 12: Properties of each modifier.

Id	Name	SBO
species_5	CAR1	

Product

Table 13: Properties of each product.

Id	Name	SBO
species_6	ERK2	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \mathrm{vol}\,(\mathrm{compartment\_1}) \cdot \mathrm{parameter\_4} \cdot [\mathrm{species\_5}] \tag{10}$$

6.6 Reaction reaction_5

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

Name k6

Reaction equation

$$\mathrm{species\_6} \xrightarrow{\mathrm{species\_2}} \emptyset \tag{11}$$

Reactant

Table 14: Properties of each reactant.

Id	Name	SBO
species_6	ERK2	

Modifier

Table 15: Properties of each modifier.

Id	Name	SBO
species_2	PKA	

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \mathrm{vol}\,(\mathrm{compartment\_1}) \cdot \mathrm{parameter\_5} \cdot [\mathrm{species\_6}] \cdot [\mathrm{species\_2}] \tag{12}$$

6.7 Reaction reaction_6

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

Name k7

Reaction equation

$$\emptyset \longrightarrow \text{species\_3} \tag{13}$$

Product

Table 16: Properties of each product.

Id	Name	SBO
species_3	REGA	

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \text{vol}\left(\text{compartment\_1}\right) \cdot \text{parameter\_6} \tag{14}$$

6.8 Reaction reaction_7

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

Name k8

Reaction equation

$$\text{species\_3} \xrightarrow{\text{species\_6}} \emptyset \tag{15}$$

Reactant

Table 17: Properties of each reactant.

Id	Name	SBO
species_3	REGA	

Modifier

Table 18: Properties of each modifier.

Id	Name	SBO
species_6	ERK2	

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \mathrm{vol}(\mathrm{compartment\_1}) \cdot \mathrm{parameter\_7} \cdot [\mathrm{species\_3}] \cdot [\mathrm{species\_6}] \tag{16}$$

6.9 Reaction reaction_8

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

Name k9

Reaction equation

$$\emptyset \xrightarrow{\mathrm{species\_4}} \mathrm{species\_1} \tag{17}$$

Modifier

Table 19: Properties of each modifier.

Id	Name	SBO
species_4	ACA	

Product

Table 20: Properties of each product.

Id	Name	SBO
species_1	In_cAMP	

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \mathrm{vol}(\mathrm{compartment\_1}) \cdot \mathrm{parameter\_8} \cdot [\mathrm{species\_4}] \tag{18}$$

6.10 Reaction reaction_9

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

Name k10

Reaction equation

$$\text{species\_1} \xrightarrow{\text{species\_3}} \emptyset \tag{19}$$

Reactant

Table 21: Properties of each reactant.

Id	Name	SBO
species_1	In_cAMP	

Modifier

Table 22: Properties of each modifier.

Id	Name	SBO
species_3	REGA	

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = \text{vol}\left(\text{compartment\_1}\right) \cdot \text{parameter\_9} \cdot [\text{species\_1}] \cdot [\text{species\_3}] \tag{20}$$

6.11 Reaction reaction_10

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

Name k11

Reaction equation

$$\emptyset \xrightarrow{\text{species\_4}} \text{species\_0} \tag{21}$$

Modifier

Table 23: Properties of each modifier.

Id	Name	SBO
species_4	ACA	

Product

Table 24: Properties of each product.

Id	Name	SBO
species_0	Ex_cAMP	

Kinetic Law

Derived unit contains undeclared units

$$v_{11} = \mathrm{vol}\,(\mathrm{compartment\_0}) \cdot \mathrm{parameter\_10} \cdot [\mathrm{species\_4}] \tag{22}$$

6.12 Reaction reaction_11

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

Name k12

Reaction equation

$$\mathrm{species\_0} \longrightarrow \emptyset \tag{23}$$

Reactant

Table 25: Properties of each reactant.

Id	Name	SBO
species_0	Ex_cAMP	

Kinetic Law

Derived unit contains undeclared units

$$v_{12} = \mathrm{vol}\,(\mathrm{compartment\_0}) \cdot \mathrm{parameter\_11} \cdot [\mathrm{species\_0}] \tag{24}$$

6.13 Reaction reaction_12

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

Name k13

Reaction equation

$$\emptyset \xrightarrow{\text{species\_0}} \text{species\_5} \tag{25}$$

Modifier

Table 26: Properties of each modifier.

Id	Name	SBO
species_0	Ex_cAMP	

Product

Table 27: Properties of each product.

Id	Name	SBO
species_5	CAR1	

Kinetic Law

Derived unit contains undeclared units

$$v_{13} = \text{vol}(\text{compartment\_1}) \cdot \text{parameter\_12} \cdot [\text{species\_0}] \tag{26}$$

6.14 Reaction reaction_13

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

Name k14

Reaction equation

$$\text{species\_5} \xrightarrow{\text{species\_2}} \emptyset \tag{27}$$

Reactant

Table 28: Properties of each reactant.

Id	Name	SBO
species_5	CAR1	

Modifier

Table 29: Properties of each modifier.

Id	Name	SBO
species_2	PKA	

Kinetic Law

Derived unit contains undeclared units

$$v_{14} = \mathrm{vol}\,(\mathrm{compartment\_1}) \cdot \mathrm{parameter\_13} \cdot [\mathrm{species\_5}] \cdot [\mathrm{species\_2}] \tag{28}$$

7 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.

7.1 Species species_0

Name Ex_cAMP

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

This species takes part in three reactions (as a reactant in reaction_11 and as a product in reaction_10 and as a modifier in reaction_12).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_0} = v_{11} - v_{12} \tag{29}$$

7.2 Species species_1

Name In_cAMP

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

This species takes part in three reactions (as a reactant in reaction_9 and as a product in reaction_8 and as a modifier in reaction_2).

$$\frac{\text{d}}{\text{d}t}\text{species\_1} = v_9 - v_{10} \tag{30}$$

7.3 Species species_2

Name PKA

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

This species takes part in four reactions (as a reactant in reaction_3 and as a product in reaction_2 and as a modifier in reaction_5, reaction_13).

$$\frac{\text{d}}{\text{d}t}\text{species\_2} = v_3 - v_4 \tag{31}$$

7.4 Species species_3

Name REGA

Initial concentration $2.5\ \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in three reactions (as a reactant in reaction_7 and as a product in reaction_6 and as a modifier in reaction_9).

$$\frac{\text{d}}{\text{d}t}\text{species\_3} = v_7 - v_8 \tag{32}$$

7.5 Species species_4

Name ACA

Initial concentration $1.4\ \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in four reactions (as a reactant in reaction_1 and as a product in reaction_0 and as a modifier in reaction_8, reaction_10).

$$\frac{\text{d}}{\text{d}t}\text{species\_4} = v_1 - v_2 \tag{33}$$

7.6 Species species_5

Name CAR1

Initial concentration $1.5\ \mu\text{mol}\cdot\text{l}^{-1}$

This species takes part in three reactions (as a reactant in reaction_13 and as a product in reaction_12 and as a modifier in reaction_4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_5} = v_{13} - v_{14} \tag{34}$$

7.7 Species species_6

Name ERK2

Initial concentration $1.6\ \mu\text{mol}\cdot\text{l}^{-1}$

This species takes part in four reactions (as a reactant in reaction_5 and as a product in reaction_4 and as a modifier in reaction_0, reaction_7).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_6} = v_{5} - v_{6} \tag{35}$$

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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