SBML Model Report

Model name: "Bindschadler2001_coupled_Ca_oscillators"

May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 1 format. This model was created by Harish Dharuri[1] at May 31st 2006 at 8:28 a. m. and last time modified at May 24th 2014 at 4:17 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	4
events	0	constraints	0
reactions	11	function definitions	0
global parameters	16	unit definitions	1
rules	8	initial assignments	0

Model Notes

The model reproduces the same amplitude antiphase calcium oscillations of coupled cells depicted in Figure 5B of the publication. This model was successfully tested on Jarnac and MathSBML. The values of „h1„ and „h2„ are not given in the publication, but the antiphase oscillations are reproduced over a narrow range of values of h1, h2,c1,c2,D and p. The values of D and p are given, while the other values were plugged in, in order to simulate the time profiles shown in the

[1]California Institute of Technology, hdharuri@cds.caltech.edu

Figure. The time t=0 in the figure may have been fixed after the system was allowed to settle, and hence does not correspond to the t=0 of the simulation.

To cite BioModels Database, please use: Li C, Donizelli M, Rodriguez N, Dharuri H, Endler L, Chelliah V, Li L, He E, Henry A, Stefan MI, Snoep JL, Hucka M, Le Novre N, Laibe C (2010) BioModels Database: An enhanced, curated and annotated resource for published quantitative kinetic models. BMC Syst Biol., 4:92.

2 Unit Definitions

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

2.1 Unit `substance`

Name micromole

Definition μmol

2.2 Unit `volume`

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

Definition l

2.3 Unit `area`

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

Definition m^2

2.4 Unit `length`

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

Definition m

2.5 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
`compartment`			3	1	litre	☑	

3.1 Compartment `compartment`

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

4 Species

This model contains four species. 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
c1	Calcium ion Cell1	compartment	$\mu mol \cdot l^{-1}$	⊟	⊟
h1	Receptor fraction Cell1	compartment	$\mu mol \cdot l^{-1}$	⊟	⊟
c2	Calcium ion Cell2	compartment	$\mu mol \cdot l^{-1}$	⊟	⊟
h2	Receptor fraction Cell2	compartment	$\mu mol \cdot l^{-1}$	⊟	⊟

5 Parameters

This model contains 16 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Phi1_c1			0.0		☐
r2			100.0		☑
R1			6.0		☑
Phi_minus1_c1			0.0		☐
k1			44.0		☑
R3			50.0		☑
Phi2_c1			0.0		☐
k2			26.5		☑
r4			20.0		☑
Phi3_c1			0.0		☐
k3			1.6		☑
R5			1.6		☑
Phi1_c2			0.0		☐
Phi_minus1_c2			0.0		☐
Phi2_c2			0.0		☐
Phi3_c2			0.0		☐

6 Rules

This is an overview of eight rules.

6.1 Rule Phi1_c1

Rule Phi1_c1 is an assignment rule for parameter Phi1_c1:

$$\text{Phi1\_c1} = \frac{\text{r2} \cdot [\text{c1}]}{\text{R1} + [\text{c1}]} \tag{1}$$

6.2 Rule Phi_minus1_c1

Rule Phi_minus1_c1 is an assignment rule for parameter Phi_minus1_c1:

$$\text{Phi\_minus1\_c1} = \frac{\text{k1}}{\text{R3} + [\text{c1}]} \tag{2}$$

6.3 Rule Phi2_c1

Rule Phi2_c1 is an assignment rule for parameter Phi2_c1:

$$\text{Phi2\_c1} = \frac{\text{k2} + \text{r4} \cdot [\text{c1}]}{\text{R3} + [\text{c1}]} \tag{3}$$

6.4 Rule Phi3_c1

Rule Phi3_c1 is an assignment rule for parameter Phi3_c1:

$$\text{Phi3\_c1} = \frac{\text{k3}}{\text{R5} + [\text{c1}]} \tag{4}$$

6.5 Rule Phi1_c2

Rule Phi1_c2 is an assignment rule for parameter Phi1_c2:

$$\text{Phi1\_c2} = \frac{\text{r2} \cdot [\text{c2}]}{\text{R1} + [\text{c2}]} \tag{5}$$

6.6 Rule Phi_minus1_c2

Rule Phi_minus1_c2 is an assignment rule for parameter Phi_minus1_c2:

$$\text{Phi\_minus1\_c2} = \frac{\text{k1}}{\text{R3} + [\text{c2}]} \tag{6}$$

6.7 Rule Phi2_c2

Rule Phi2_c2 is an assignment rule for parameter Phi2_c2:

$$\text{Phi2\_c2} = \frac{\text{k2} + \text{r4} \cdot [\text{c2}]}{\text{R3} + [\text{c2}]} \tag{7}$$

6.8 Rule Phi3_c2

Rule Phi3_c2 is an assignment rule for parameter Phi3_c2:

$$\text{Phi3\_c2} = \frac{\text{k3}}{\text{R5} + [\text{c2}]} \tag{8}$$

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	Jreceptor_Cell1	IP3R mediated Ca release Cell1	$\emptyset \xrightarrow{h1} c1$	
2	Jpump_Cell1	ATPase pump mediated Ca efflux Cell1	$c1 \longrightarrow \emptyset$	
3	Jleak_Cell1	IP3R independent Ca release Cell1	$\emptyset \longrightarrow c1$	
4	Inactivated_to_S_Cell1	Inactivated to Shut state transition Cell1	$\emptyset \longrightarrow h1$	
5	Open_to_Inactivated_Cell1	Open to Inactivated state transition Cell1	$h1 \longrightarrow \emptyset$	
6	Jreceptor_Cell2	IP3R mediated Ca release Cell2	$\emptyset \xrightarrow{h2} c2$	
7	Jpump_Cell2	ATPase pump mediated Ca efflux Cell2	$c2 \longrightarrow \emptyset$	
8	Jleak_Cell2	IP3R independent Ca release Cell2	$\emptyset \longrightarrow c2$	
9	Inactivated_to_S_Cell2	Inactivated to Shut state transition Cell2	$\emptyset \longrightarrow h2$	
10	Open_to_Inactivated_Cell2	Open to Inactivated state transition Cell2	$h2 \longrightarrow \emptyset$	
11	diffusion	Diffusion of Ca between cells	$c2 \longrightarrow c1$	

7.1 Reaction Jreceptor_Cell1

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

Name IP3R mediated Ca release Cell1

Reaction equation

$$\emptyset \xrightarrow{\text{h1}} \text{c1} \tag{9}$$

Modifier

Table 6: Properties of each modifier.

Id	Name	SBO
h1	Receptor fraction Cell1	

Product

Table 7: Properties of each product.

Id	Name	SBO
c1	Calcium ion Cell1	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \text{vol}\,(\text{compartment}) \cdot \text{kf} \cdot \left(\frac{\text{p} \cdot [\text{h1}] \cdot \text{Phi1\_c1}}{\text{Phi1\_c1} \cdot \text{p} + \text{Phi\_minus1\_c1}} \right)^4 \tag{10}$$

Table 8: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
kf			28.000		☑
p			0.278		☑

7.2 Reaction Jpump_Cell1

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

Name ATPase pump mediated Ca efflux Cell1

Reaction equation

$$\mathrm{c1} \longrightarrow \emptyset \tag{11}$$

Reactant

Table 9: Properties of each reactant.

Id	Name	SBO
c1	Calcium ion Cell1	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \frac{\mathrm{Vp} \cdot [\mathrm{c1}]^2}{\mathrm{Kp}^2 + [\mathrm{c1}]^2} \tag{12}$$

Table 10: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vp			1.20		☑
Kp			0.18		☑

7.3 Reaction Jleak_Cell1

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

Name IP3R independent Ca release Cell1

Reaction equation

$$\emptyset \longrightarrow \mathrm{c1} \tag{13}$$

Product

Table 11: Properties of each product.

Id	Name	SBO
c1	Calcium ion Cell1	

Id	Name	SBO

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{Jleak} \tag{14}$$

Table 12: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
`Jleak`			0.2		☑

7.4 Reaction `Inactivated_to_S_Cell1`

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

Name Inactivated to Shut state transition Cell1

Reaction equation

$$\emptyset \longrightarrow \mathrm{h1} \tag{15}$$

Product

Table 13: Properties of each product.

Id	Name	SBO
`h1`	Receptor fraction Cell1	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{Phi3\_c1} \cdot (1 - [\mathrm{h1}]) \tag{16}$$

7.5 Reaction `Open_to_Inactivated_Cell1`

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

Name Open to Inactivated state transition Cell1

Reaction equation

$$\mathrm{h1} \longrightarrow \emptyset \tag{17}$$

Reactant

Table 14: Properties of each reactant.

Id	Name	SBO
h1	Receptor fraction Cell1	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \frac{\mathrm{vol\,(compartment)} \cdot \mathrm{Phi1\_c1} \cdot \mathrm{Phi2\_c1} \cdot [\mathrm{h1}] \cdot \mathrm{p}}{\mathrm{Phi1\_c1} \cdot \mathrm{p} + \mathrm{Phi\_minus1\_c1}} \tag{18}$$

Table 15: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
p			0.278		☑

7.6 Reaction Jreceptor_Cell2

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

Name IP3R mediated Ca release Cell2

Reaction equation

$$\emptyset \xrightarrow{\mathrm{h2}} \mathrm{c2} \tag{19}$$

Modifier

Table 16: Properties of each modifier.

Id	Name	SBO
h2	Receptor fraction Cell2	

Product

Table 17: Properties of each product.

Id	Name	SBO
c2	Calcium ion Cell2	

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{kf} \cdot \left(\frac{\mathrm{p} \cdot [\mathrm{h2}] \cdot \mathrm{Phi1\_c2}}{\mathrm{Phi1\_c2} \cdot \mathrm{p} + \mathrm{Phi\_minus1\_c2}} \right)^4 \tag{20}$$

Table 18: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
kf			28.000		☑
p			0.278		☑

7.7 Reaction Jpump_Cell2

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

Name ATPase pump mediated Ca efflux Cell2

Reaction equation

$$\mathrm{c2} \longrightarrow \emptyset \tag{21}$$

Reactant

Table 19: Properties of each reactant.

Id	Name	SBO
c2	Calcium ion Cell2	

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \frac{\mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{Vp} \cdot [\mathrm{c2}]^2}{\mathrm{Kp}^2 + [\mathrm{c2}]^2} \tag{22}$$

Table 20: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vp			1.20		☑
Kp			0.18		☑

7.8 Reaction Jleak_Cell2

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

Name IP3R independent Ca release Cell2

Reaction equation

$$\emptyset \longrightarrow \mathrm{c2} \tag{23}$$

Product

Table 21: Properties of each product.

Id	Name	SBO
c2	Calcium ion Cell2	

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{Jleak} \tag{24}$$

Table 22: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Jleak			0.2		☑

7.9 Reaction Inactivated_to_S_Cell2

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

Name Inactivated to Shut state transition Cell2

Reaction equation

$$\emptyset \longrightarrow \mathrm{h2} \tag{25}$$

Product

Table 23: Properties of each product.

Id	Name	SBO
h2	Receptor fraction Cell2	

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{Phi3\_c2} \cdot (1 - [\mathrm{h2}]) \tag{26}$$

7.10 Reaction Open_to_Inactivated_Cell2

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

Name Open to Inactivated state transition Cell2

Reaction equation

$$\mathrm{h2} \longrightarrow \emptyset \tag{27}$$

Reactant

Table 24: Properties of each reactant.

Id	Name	SBO
h2	Receptor fraction Cell2	

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = \frac{\mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{Phi1\_c2} \cdot \mathrm{Phi2\_c2} \cdot [\mathrm{h2}] \cdot \mathrm{p}}{\mathrm{Phi1\_c2} \cdot \mathrm{p} + \mathrm{Phi\_minus1\_c2}} \tag{28}$$

Table 25: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
p			0.278		☑

7.11 Reaction `diffusion`

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

Name Diffusion of Ca between cells

Reaction equation

$$\mathrm{c2} \longrightarrow \mathrm{c1} \tag{29}$$

Reactant

Table 26: Properties of each reactant.

Id	Name	SBO
c2	Calcium ion Cell2	

Product

Table 27: Properties of each product.

Id	Name	SBO
c1	Calcium ion Cell1	

Kinetic Law

Derived unit contains undeclared units

$$v_{11} = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{D} \cdot ([\mathrm{c2}] - [\mathrm{c1}]) \tag{30}$$

Table 28: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
D			0.01		☑

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.

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.

8.1 Species `c1`

Name Calcium ion Cell1

Initial concentration $0.3\ \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in four reactions (as a reactant in `Jpump_Cell1` and as a product in `Jreceptor_Cell1`, `Jleak_Cell1`, `diffusion`).

$$\frac{\text{d}}{\text{d}t}\text{c1} = v_1 + v_3 + v_{11} - v_2 \tag{31}$$

8.2 Species `h1`

Name Receptor fraction Cell1

Initial concentration $0.8\ \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in three reactions (as a reactant in `Open_to_Inactivated_Cell1` and as a product in `Inactivated_to_S_Cell1` and as a modifier in `Jreceptor_Cell1`).

$$\frac{\text{d}}{\text{d}t}\text{h1} = v_4 - v_5 \tag{32}$$

8.3 Species `c2`

Name Calcium ion Cell2

Initial concentration $0.1\ \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in four reactions (as a reactant in `Jpump_Cell2`, `diffusion` and as a product in `Jreceptor_Cell2`, `Jleak_Cell2`).

$$\frac{\text{d}}{\text{d}t}\text{c2} = v_6 + v_8 - v_7 - v_{11} \tag{33}$$

8.4 Species h2

Name Receptor fraction Cell2

Initial concentration $0.1\ \mu\text{mol}\cdot\text{l}^{-1}$

This species takes part in three reactions (as a reactant in Open_to_Inactivated_Cell2 and as a product in Inactivated_to_S_Cell2 and as a modifier in Jreceptor_Cell2).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{h2} = v_9 - v_{10} \tag{34}$$

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.

[a]Center for Bioinformatics Tübingen (ZBIT), Germany
[b]California Institute of Technology, Beckman Institute BNMC, Pasadena, United States
[c]European Bioinformatics Institute, Wellcome Trust Genome Campus, Hinxton, United Kingdom
[d]EML Research gGmbH, Heidelberg, Germany