SBML Model Report

Model name: “Oxhamre2005_Ca_oscillation”

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 August 25th 2005 at eleven o’ clock in the morning. and last time modified at March 26th 2014 at 5:37 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	2
species types	0	species	2
events	0	constraints	0
reactions	3	function definitions	0
global parameters	13	unit definitions	2
rules	4	initial assignments	0

Model Notes

The model should reproduce the figure 1C of the article (successfully reproduced in MathSBML). If your software does not support the variable „time„, you can replace the assignmentRule:
n = n0 * [exp(-kbN*time) + kappa * (1 - exp(-kbN*time))]
by
n = n0 * kappa

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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 `substance`

Name micromole (default)

Definition µmol

2.2 Unit `time`

Name minute (default)

Definition 60 s

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
Cytosol			3	1	litre	☑	
Endoplasmic_Reticulum			3	1	litre	☑	Cytosol

3.1 Compartment Cytosol

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

3.2 Compartment Endoplasmic_Reticulum

This is a three dimensional compartment with a constant size of one litre, which is surrounded by Cytosol.

4 Species

This model contains two 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
CaER		Endoplasmic_Reticulum	$\mu mol \cdot l^{-1}$	⊟	⊟
Ca_Cyt		Cytosol	$\mu mol \cdot l^{-1}$	⊟	⊟

5 Parameters

This model contains 13 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
n			1.00		☐
n0			1.00		☑
kbN			0.50		☑
kappa			5.00		☑
p1			0.00		☐
p11			0.20		☑
p12			0.80		☑
K1			5.00		☑
p2			0.00		☐
K2			0.70		☑
p3			0.95		☐
k31			0.50		☑
K3			0.70		☑

6 Rules

This is an overview of four rules.

6.1 Rule n

Rule n is an assignment rule for parameter n:

$$\mathrm{n} = \mathrm{n0} \cdot (\exp(\mathrm{kbN} \cdot \mathrm{Time}) + \mathrm{kappa} \cdot (1 - \exp(\mathrm{kbN} \cdot \mathrm{Time}))) \tag{1}$$

6.2 Rule p1

Rule p1 is an assignment rule for parameter p1:

$$\mathrm{p1} = \mathrm{p11} + \frac{\mathrm{p12} \cdot \mathrm{n}}{\mathrm{K1} + \mathrm{n}} \tag{2}$$

6.3 Rule p2

Rule p2 is an assignment rule for parameter p2:

$$\mathrm{p2} = \frac{[\mathrm{Ca\_Cyt}]}{\mathrm{K2} + [\mathrm{Ca\_Cyt}]} \tag{3}$$

6.4 Rule p3

Rule p3 is a rate rule for parameter p3:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{p3} = (\mathrm{k31} \cdot [\mathrm{Ca\_Cyt}] \cdot \mathrm{p3}) + \mathrm{k31} \cdot \mathrm{K3} \cdot (1 - \mathrm{p3}) \tag{4}$$

7 Reactions

This model contains three 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	Jch		CaER ⟶ Ca_Cyt	
2	Jleak		CaER ⟶ Ca_Cyt	
3	Jpump		Ca_Cyt ⟶ CaER	

7.1 Reaction Jch

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

Reaction equation

$$\text{CaER} \longrightarrow \text{Ca\_Cyt} \tag{5}$$

Reactant

Table 6: Properties of each reactant.

Id	Name	SBO
CaER		

Product

Table 7: Properties of each product.

Id	Name	SBO
Ca_Cyt		

Kinetic Law

Derived unit not available

$$v_1 = \text{Fch\_0} \cdot \text{p1} \cdot \text{p2} \cdot \text{p3} \tag{6}$$

Table 8: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Fch_0			8.0		☑

7.2 Reaction Jleak

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

Reaction equation

$$\text{CaER} \longrightarrow \text{Ca\_Cyt} \tag{7}$$

Reactant

Table 9: Properties of each reactant.

Id	Name	SBO
CaER		

Product

Table 10: Properties of each product.

Id	Name	SBO
Ca_Cyt		

Kinetic Law

Derived unit not available

$$v_2 = \text{Fleak} \tag{8}$$

Table 11: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Fleak			0.5		☑

7.3 Reaction Jpump

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

Reaction equation

$$\text{Ca\_Cyt} \longrightarrow \text{CaER} \tag{9}$$

Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
Ca_Cyt		

Product

Table 13: Properties of each product.

Id	Name	SBO
CaER		

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \frac{\text{Fpump\_0} \cdot [\text{Ca\_Cyt}]}{\text{Kpump} + [\text{Ca\_Cyt}]} \tag{10}$$

Table 14: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Fpump_0			2.0		☑
Kpump			0.1		☑

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 CaER

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

This species takes part in three reactions (as a reactant in Jch, Jleak and as a product in Jpump).

$$\frac{\text{d}}{\text{d}t}\text{CaER} = v_3 - v_1 - v_2 \tag{11}$$

8.2 Species Ca_Cyt

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

This species takes part in three reactions (as a reactant in Jpump and as a product in Jch, Jleak).

$$\frac{\text{d}}{\text{d}t}\text{Ca\_Cyt} = v_1 + v_2 - v_3 \tag{12}$$

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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