SBML Model Report

Model name: "Marhl2000_CaOscillations"

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1 General Overview

This is a document in SBML Level 2 Version 1 format. This model was created by the following two authors: Nicolas Le Novre[1] and Harish Dharuri[2] at July 15th 2005 at 9:10 a. m. and last time modified at February twelveth 2014 at 2:17 p. 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	3
species types	0	species	5
events	0	constraints	0
reactions	7	function definitions	0
global parameters	0	unit definitions	1
rules	0	initial assignments	0

Model Notes

In order to reproduce the model, the volume of all compartment is set to 1, and the stoichiometry of CaER and CaM has been set to 0.25, corresponding to betaER/rhoER and betaM/rhoM described in the paper.

[1]EMBL-EBI, lenov@ebi.ac.uk
[2]Keck Graduate Institute, Harish_Dharuri@kgi.edu

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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 (default)

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 Compartments

This model contains three 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
Mitochondria			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.

3.3 Compartment Mitochondria

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

4 Species

This model contains five 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
Ca_cyt		Cytosol	$\mu mol \cdot l^{-1}$	⊟	⊟
CaER		Endoplasmic_Reticulum	$\mu mol \cdot l^{-1}$	⊟	⊟
CaM		Mitochondria	$\mu mol \cdot l^{-1}$	⊟	⊟
CaPr		Cytosol	$\mu mol \cdot l^{-1}$	⊟	⊟
Pr		Cytosol	$\mu mol \cdot l^{-1}$	⊟	⊟

5 Reactions

This model contains seven 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	v1	Jch	$0 \cdot 25\,\mathrm{CaER} \xrightarrow{\mathrm{Ca\_cyt}} \mathrm{Ca\_cyt}$	
2	v3	Jleak	$0 \cdot 25\,\mathrm{CaER} \longrightarrow \mathrm{Ca\_cyt}$	
3	v5	Jpump	$\mathrm{Ca\_cyt} \longrightarrow 0 \cdot 25\,\mathrm{CaER}$	
4	v7	Jout	$0 \cdot 25\,\mathrm{CaM} \xrightarrow{\mathrm{Ca\_cyt}} \mathrm{Ca\_cyt}$	
5	v9	Jin	$\mathrm{Ca\_cyt} \xrightarrow{\mathrm{Ca\_cyt}} 0 \cdot 25\,\mathrm{CaM}$	
6	v11	dissociation of CaPr	$\mathrm{CaPr} \longrightarrow \mathrm{Pr} + \mathrm{Ca\_cyt}$	
7	v12	binding of Ca on Pr	$\mathrm{Pr} + \mathrm{Ca\_cyt} \longrightarrow \mathrm{CaPr}$	

5.1 Reaction v1

This is an irreversible reaction of one reactant forming one product influenced by one modifier.

Name Jch

Reaction equation

$$0{\cdot}25\,\mathrm{CaER} \xrightarrow{\mathrm{Ca\_cyt}} \mathrm{Ca\_cyt} \tag{1}$$

Reactant

Table 5: Properties of each reactant.

Id	Name	SBO
CaER		

Modifier

Table 6: Properties of each modifier.

Id	Name	SBO
Ca_cyt		

Product

Table 7: Properties of each product.

Id	Name	SBO
Ca_cyt		

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \mathrm{vol}\,(\mathrm{Cytosol}) \cdot \frac{\mathrm{Kch} \cdot [\mathrm{Ca\_cyt}]^2 \cdot ([\mathrm{CaER}] - [\mathrm{Ca\_cyt}])}{\mathrm{K1}^2 + [\mathrm{Ca\_cyt}]^2} \tag{2}$$

Table 8: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Kch			4100.0		☑
K1			5.0		☑

5.2 Reaction v3

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

Name Jleak

Reaction equation

$$0{\cdot}25\,\mathrm{CaER} \longrightarrow \mathrm{Ca\_cyt} \tag{3}$$

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 contains undeclared units

$$v_2 = \mathrm{vol}\,(\mathrm{Cytosol}) \cdot \mathrm{Kleak} \cdot ([\mathrm{CaER}] - [\mathrm{Ca\_cyt}]) \tag{4}$$

Table 11: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Kleak			0.05		☑

5.3 Reaction v5

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

Name Jpump

Reaction equation

$$\text{Ca\_cyt} \longrightarrow 0{\cdot}25\,\text{CaER} \tag{5}$$

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

$$v_3 = \text{vol}\left(\text{Endoplasmic\_Reticulum}\right) \cdot \text{Kpump} \cdot [\text{Ca\_cyt}] \tag{6}$$

Table 14: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Kpump			20.0		☑

5.4 Reaction v7

This is an irreversible reaction of one reactant forming one product influenced by one modifier.

Name Jout

Reaction equation

$$0{\cdot}25\,\mathrm{CaM} \xrightarrow{\mathrm{Ca\_cyt}} \mathrm{Ca\_cyt} \tag{7}$$

Reactant

Table 15: Properties of each reactant.

Id	Name	SBO
CaM		

Modifier

Table 16: Properties of each modifier.

Id	Name	SBO
Ca_cyt		

Product

Table 17: Properties of each product.

Id	Name	SBO
Ca_cyt		

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \mathrm{vol}\,(\mathrm{Cytosol}) \cdot [\mathrm{CaM}] \cdot \left(\frac{\mathrm{Kout} \cdot [\mathrm{Ca\_cyt}]^2}{\mathrm{K3}^2 + [\mathrm{Ca\_cyt}]^2} + \mathrm{Km} \right) \tag{8}$$

Table 18: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Kout			125.000		☑
K3			5.000		☑
Km			0.006		☑

5.5 Reaction v9

This is an irreversible reaction of one reactant forming one product influenced by one modifier.

Name Jin

Reaction equation

$$\mathrm{Ca\_cyt} \xrightarrow{\mathrm{Ca\_cyt}} 0{\cdot}25\,\mathrm{CaM} \tag{9}$$

Reactant

Table 19: Properties of each reactant.

Id	Name	SBO
Ca_cyt		

Modifier

Table 20: Properties of each modifier.

Id	Name	SBO
Ca_cyt		

Product

Table 21: Properties of each product.

Id	Name	SBO
CaM		

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \mathrm{vol}\,(\mathrm{Mitochondria}) \cdot \frac{\mathrm{Kin} \cdot [\mathrm{Ca\_cyt}]^8}{\mathrm{K2}^8 + [\mathrm{Ca\_cyt}]^8} \tag{10}$$

Table 22: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Kin			300.0		☑
K2			0.8		☑

5.6 Reaction v11

This is an irreversible reaction of one reactant forming two products.

Name dissociation of CaPr

Reaction equation

$$\mathrm{CaPr} \longrightarrow \mathrm{Pr} + \mathrm{Ca\_cyt} \tag{11}$$

Reactant

Table 23: Properties of each reactant.

Id	Name	SBO
CaPr		

Products

Table 24: Properties of each product.

Id	Name	SBO
Pr		
Ca_cyt		

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \mathrm{vol}\left(\mathrm{Cytosol}\right) \cdot \mathrm{Kminus} \cdot [\mathrm{CaPr}] \tag{12}$$

Table 25: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Kminus			0.01		☑

5.7 Reaction v12

This is an irreversible reaction of two reactants forming one product.

Name binding of Ca on Pr

Reaction equation

$$\mathrm{Pr} + \mathrm{Ca\_cyt} \longrightarrow \mathrm{CaPr} \tag{13}$$

Reactants

Table 26: Properties of each reactant.

Id	Name	SBO
Pr		
Ca_cyt		

Product

Table 27: Properties of each product.

Id	Name	SBO
CaPr		

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \mathrm{vol}\,(\mathrm{Cytosol}) \cdot \mathrm{Kplus} \cdot [\mathrm{Ca\_cyt}] \cdot [\mathrm{Pr}] \tag{14}$$

Table 28: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Kplus			0.1		☑

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 `Ca_cyt`

Initial concentration $0.35\ \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in ten reactions (as a reactant in `v5`, `v9`, `v12` and as a product in `v1`, `v3`, `v7`, `v11` and as a modifier in `v1`, `v7`, `v9`).

$$\frac{\text{d}}{\text{d}t}\text{Ca\_cyt} = v_1 + v_2 + v_4 + v_6 - v_3 - v_5 - v_7 \tag{15}$$

6.2 Species `CaER`

Initial concentration $0.76\ \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in three reactions (as a reactant in `v1`, `v3` and as a product in `v5`).

$$\frac{\text{d}}{\text{d}t}\text{CaER} = 0.25\, v_3 - 0.25\, v_1 - 0.25\, v_2 \tag{16}$$

6.3 Species `CaM`

Initial concentration $0.29\ \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a reactant in `v7` and as a product in `v9`).

$$\frac{\text{d}}{\text{d}t}\text{CaM} = 0.25\, v_5 - 0.25\, v_4 \tag{17}$$

6.4 Species `CaPr`

Initial concentration $85.45\ \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a reactant in `v11` and as a product in `v12`).

$$\frac{\text{d}}{\text{d}t}\text{CaPr} = v_7 - v_6 \tag{18}$$

6.5 Species `Pr`

Initial concentration $34.55\ \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a reactant in `v12` and as a product in `v11`).

$$\frac{\text{d}}{\text{d}t}\text{Pr} = v_6 - v_7 \tag{19}$$

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