SBML Model Report

Model name: “Somogyi1990_CaOscillations”

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1 General Overview

This is a document in SBML Level 2 Version 1 format. This model was created by Enuo He[1] at May tenth 2007 at 8:46 a. m. and last time modified at April sixth 2014 at 10:01 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	3
species types	0	species	2
events	0	constraints	0
reactions	4	function definitions	0
global parameters	8	unit definitions	0
rules	1	initial assignments	0

Model Notes

This model encoded according to the paper *Hormone induced Calcium Oscillations in Liver Cells Can Be Explained by a Simple One Pool Model.* The values of parameters a and alpha are varioused inorder to simulate results in different situations. For Figure 3A, a=3.5,alpha=1.2 ; Figure 3B, a=3,alpha=5 ; Figure 3C a= 0.95, alpha=1.5; Figure3D, a=1, alpha=5. Keep in mind that the value for the xy axies are arbitrary value. Figures3 in the paper are reproduced by COPASI 4.0.20(development) , and SBMLodeSolver online.

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2 Unit Definitions

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

2.1 Unit `substance`

Notes Mole is the predefined SBML unit for `substance`.

Definition mol

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
cytoplasm			3	1	litre	☑	
ER	endoplasmic reticulum		3	1	litre	☑	
extracellular			3	1	litre	☑	

3.1 Compartment cytoplasm

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

3.2 Compartment ER

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

Name endoplasmic reticulum

3.3 Compartment extracellular

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

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
x	Ca_ER	ER	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
y	Ca_Cyt	cytoplasm	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟

5 Parameters

This model contains eight global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k			0.01		☑
alpha			5.00		☑
n			4.00		☑
a			3.00		☑
k1			2.00		☑
beta			1.00		☑
fy			0.00		☐
gamma			1.00		☑

6 Rule

This is an overview of one rule.

6.1 Rule fy

Rule fy is an assignment rule for parameter fy:

$$\mathrm{fy} = \frac{[\mathrm{y}]^{\mathrm{n}}}{\mathrm{a}^{\mathrm{n}} + [\mathrm{y}]^{\mathrm{n}}} \tag{1}$$

7 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 5: Overview of all reactions

№	Id	Name	Reaction Equation	SBO
1	reaction_0000001	Ca flux into the cell	$\emptyset \longrightarrow y$	
2	reaction_0000002	Ca translocation between cytoplasm and ER	$x \rightleftharpoons y$	
3	reaction_0000003	Ca pumped out of the cell	$y \longrightarrow \emptyset$	
4	reaction_0000004	InsP3 channel	$x \longrightarrow y$	

7.1 Reaction reaction_0000001

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

Name Ca flux into the cell

Reaction equation

$$\emptyset \longrightarrow \mathrm{y} \tag{2}$$

Product

Table 6: Properties of each product.

Id	Name	SBO
y	Ca_Cyt	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \mathrm{gamma} \cdot \mathrm{vol}\left(\mathrm{cytoplasm}\right) \tag{3}$$

7.2 Reaction reaction_0000002

This is a reversible reaction of one reactant forming one product.

Name Ca translocation between cytoplasm and ER

Reaction equation

$$\mathrm{x} \rightleftharpoons \mathrm{y} \tag{4}$$

Reactant

Table 7: Properties of each reactant.

Id	Name	SBO
x	Ca_ER	

Product

Table 8: Properties of each product.

Id	Name	SBO
y	Ca_Cyt	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \mathrm{k} \cdot [\mathrm{x}] \cdot \mathrm{vol}\,(\mathrm{cytoplasm}) - \mathrm{k1} \cdot [\mathrm{y}] \cdot \mathrm{vol}\,(\mathrm{ER}) \tag{5}$$

7.3 Reaction `reaction_0000003`

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

Name Ca pumped out of the cell

Reaction equation

$$\mathrm{y} \longrightarrow \emptyset \tag{6}$$

Reactant

Table 9: Properties of each reactant.

Id	Name	SBO
y	Ca_Cyt	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \mathrm{beta} \cdot [\mathrm{y}] \cdot \mathrm{vol}\,(\mathrm{extracellular}) \tag{7}$$

7.4 Reaction `reaction_0000004`

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

Name InsP3 channel

Reaction equation

$$\mathrm{x} \longrightarrow \mathrm{y} \tag{8}$$

Reactant

Table 10: Properties of each reactant.

Id	Name	SBO
x	Ca_ER	

Product

Table 11: Properties of each product.

Id	Name	SBO
y	Ca_Cyt	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \text{alpha} \cdot \text{fy} \cdot [\text{x}] \cdot \text{vol}\,(\text{cytoplasm}) \tag{9}$$

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 x

Name Ca_ER

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

This species takes part in two reactions (as a reactant in reaction_0000002, reaction_0000004).

$$\frac{\text{d}}{\text{d}t}\text{x} = -v_2 - v_4 \tag{10}$$

8.2 Species y

Name Ca_Cyt

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

This species takes part in four reactions (as a reactant in reaction_0000003 and as a product in reaction_0000001, reaction_0000002, reaction_0000004).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{y} = v_1 + v_2 + v_4 - v_3 \tag{11}$$

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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