SBML Model Report

Model name: "Larsen2004_CalciumSpiking"

May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by Vijayalakshmi Chelliah[1] at May fifth 2011 at 12:59 a. m. and last time modified at May 28th 2014 at 2:48 a. 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	5
events	0	constraints	0
reactions	0	function definitions	0
global parameters	21	unit definitions	0
rules	5	initial assignments	0

Model Notes

This model is from the article:
On the encoding and decoding of calcium signals in hepatocytes
Ann Zahle Larsen, Lars Folke Olsen and Ursula Kummera Biophysical ChemistryVolume 107, Issue 1, 1 January 2004, Pages 83-99 14871603,
Abstract:
Many different agonists use calcium as a second messenger. Despite intensive research in intracellular calcium signalling it is an unsolved riddle how the different types of information

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represented by the different agonists, is encoded using the universal carrier calcium. It is also still not clear how the information encoded is decoded again into the intracellular specific information at the site of enzymes and genes. After the discovery of calcium oscillations, one likely mechanism is that information is encoded in the frequency, amplitude and waveform of the oscillations. This hypothesis has received some experimental support. However, the mechanism of decoding of oscillatory signals is still not known. Here, we study a mechanistic model of calcium oscillations, which is able to reproduce both spiking and bursting calcium oscillations. We use the model to study the decoding of calcium signals on the basis of co-operativity of calcium binding to various proteins. We show that this co-operativity offers a simple way to decode different calcium dynamics into different enzyme activities.

Note:

This model corresponds to the 5 variable receptor-operated model, as described by Larsen et al., 2004. This model is a modified version of the model described in Kummer 2000 (PMID:10968983)

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`	cytoplasm	0000290	3	1	litre	☑	
`ER`	ER	0000290	3	1	litre	☑	
`mit`	mitochondria	0000290	3	1	litre	☑	

3.1 Compartment `cytoplasm`

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

Name cytoplasm

SBO:0000290 physical compartment

3.2 Compartment `ER`

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

Name ER

SBO:0000290 physical compartment

3.3 Compartment `mit`

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

Name mitochondria

SBO:0000290 physical compartment

4 Species

This model contains five 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
G_alpha	G-alpha	cytoplasm	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
PLC	PLC	cytoplasm	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Ca_cyt	Calcium-Cyt	cytoplasm	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Ca_ER	Calcium-ER	ER	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Ca_mit	Calcium-mit	mit	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟

5 Parameters

This model contains 21 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1	0000009	0.350		☑
k2	k2	0000009	0.000		☑
k3	k3	0000009	10^{-4}		☑
K4	K4	0000009	0.783		☑
k5	k5	0000009	1.240		☑
K6	K6	0000009	0.700		☑
k7	k7	0000009	5.820		☑
k8	k8	0000009	32.240		☑
K9	K9	0000009	29.090		☑
k10	k10	0000009	0.930		☑
K11	K11	0000009	2.667		☑
k12	k12	0000009	0.760		☑
k13	k13	0000009	0.000		☑
k14	k14	0000009	149.000		☑
K15	K15	0000009	0.160		☑
k16	k16	0000009	20.900		☑
K17	K17	0000009	0.050		☑
k18	k18	0000009	79.000		☑
K19	K19	0000009	2.000		☑
k20	k20	0000009	1.500		☑
K21	K21	0000009	1.500		☑

6 Rules

This is an overview of five rules.

6.1 Rule G_alpha

Rule G_alpha is a rate rule for species G_alpha:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{G\_alpha} = \mathrm{k1} + \mathrm{k2} \cdot [\mathrm{G\_alpha}] - \frac{\mathrm{k3} \cdot [\mathrm{G\_alpha}] \cdot [\mathrm{PLC}]}{[\mathrm{G\_alpha}] + \mathrm{K4}} - \frac{\mathrm{k5} \cdot [\mathrm{G\_alpha}] \cdot [\mathrm{Ca\_cyt}]}{[\mathrm{G\_alpha}] + \mathrm{K6}} \tag{1}$$

6.2 Rule PLC

Rule PLC is a rate rule for species PLC:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{PLC} = \mathrm{k7} \cdot [\mathrm{G\_alpha}] - \frac{\mathrm{k8} \cdot [\mathrm{PLC}]}{[\mathrm{PLC}] + \mathrm{K9}} \tag{2}$$

6.3 Rule Ca_cyt

Rule Ca_cyt is a rate rule for species Ca_cyt:

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Ca\_cyt} = &\frac{([\mathrm{Ca\_ER}] - [\mathrm{Ca\_cyt}]) \cdot \mathrm{k10} \cdot [\mathrm{Ca\_cyt}] \cdot [\mathrm{PLC}]^4}{[\mathrm{PLC}]^4 + \mathrm{K11}^4} + \mathrm{k12} \cdot [\mathrm{PLC}] \\ &+ \mathrm{k13} \cdot [\mathrm{G\_alpha}] - \frac{\mathrm{k14} \cdot [\mathrm{Ca\_cyt}]}{[\mathrm{Ca\_cyt}] + \mathrm{K15}} - \frac{\mathrm{k16} \cdot [\mathrm{Ca\_cyt}]}{[\mathrm{Ca\_cyt}] + \mathrm{K17}} \\ &- \frac{\mathrm{k18} \cdot [\mathrm{Ca\_cyt}]^8}{\mathrm{K19}^8 + [\mathrm{Ca\_cyt}]^8} + \frac{([\mathrm{Ca\_mit}] - [\mathrm{Ca\_cyt}]) \cdot \mathrm{k20} \cdot [\mathrm{Ca\_cyt}]}{[\mathrm{Ca\_cyt}] + \mathrm{K21}}\end{aligned} \tag{3}$$

6.4 Rule Ca_ER

Rule Ca_ER is a rate rule for species Ca_ER:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Ca\_ER} = \frac{([\mathrm{Ca\_ER}] - [\mathrm{Ca\_cyt}]) \cdot \mathrm{k10} \cdot [\mathrm{Ca\_cyt}] \cdot [\mathrm{PLC}]^4}{[\mathrm{PLC}]^4 + \mathrm{K11}^4} + \frac{\mathrm{k16} \cdot [\mathrm{Ca\_cyt}]}{[\mathrm{Ca\_cyt}] + \mathrm{K17}} \tag{4}$$

6.5 Rule Ca_mit

Rule Ca_mit is a rate rule for species Ca_mit:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Ca\_mit} = \frac{\mathrm{k18} \cdot [\mathrm{Ca\_cyt}]^8}{\mathrm{K19}^8 + [\mathrm{Ca\_cyt}]^8} - \frac{([\mathrm{Ca\_mit}] - [\mathrm{Ca\_cyt}]) \cdot \mathrm{k20} \cdot [\mathrm{Ca\_cyt}]}{[\mathrm{Ca\_cyt}] + \mathrm{K21}} \tag{5}$$

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.

7.1 Species G_alpha

Name G-alpha

SBO:0000252 polypeptide chain

Initial concentration $0.01\ \mathrm{mol} \cdot \mathrm{l}^{-1}$

Involved in rule G_alpha

One rule which determines this species' quantity.

7.2 Species PLC

Name PLC

SBO:0000014 enzyme

Initial amount 0.01 mol

Involved in rule PLC

One rule which determines this species' quantity.

7.3 Species Ca_cyt

Name Calcium-Cyt

SBO:0000247 simple chemical

Initial amount 0.01 mol

Involved in rule Ca_cyt

One rule which determines this species' quantity.

7.4 Species Ca_ER

Name Calcium-ER

SBO:0000247 simple chemical

Initial amount 10 mol

Involved in rule Ca_ER

One rule which determines this species' quantity.

7.5 Species Ca_mit

Name Calcium-mit

SBO:0000247 simple chemical

Initial concentration $0.0010 \text{ mol} \cdot \text{l}^{-1}$

Involved in rule Ca_mit

One rule which determines this species' quantity.

A Glossary of Systems Biology Ontology Terms

SBO:0000009 kinetic constant: Numerical parameter that quantifies the velocity of a chemical reaction

SBO:0000014 enzyme: A protein that catalyzes a chemical reaction. The word comes from en "a" or"i") and simo "leave" or"yeas")

SBO:0000247 simple chemical: Simple, non-repetitive chemical entity

SBO:0000252 polypeptide chain: Naturally occurring macromolecule formed by the repetition of amino-acid residues linked by peptidic bonds. A polypeptide chain is synthesized by the ribosome. CHEBI:1654

SBO:0000290 physical compartment: Specific location of space, that can be bounded or not. A physical compartment can have 1, 2 or 3 dimensions

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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