SBML Model Report

Model name: "Borghans1997 - Calcium Oscillation - Model 1"



May 6, 2016

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 Novre¹ and Harish Dharuri² at July eighth 2005 at 1:06 p. m. and last time modified at June third 2013 at 3:58 p. m. Table 1 shows 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	3	unit definitions	2
rules	0	initial assignments	0

Model Notes

Borghans 1997 - Calcium Oscillation - Model 1

A theoretical expoloration of possible mechanisms of intracellular calcium oscillations has been studied, considering three hypothesis (see below). This model corresponds to the first hypothesis.

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This model is described in the article:Complex intracellular calcium oscillations. A theoretical exploration of possible mechanisms.Borghans JM, Dupont G, Goldbeter A.Biophys. Chem. 1997 May; 66(1): 25-41

Abstract:

Intracellular Ca(2+) oscillations are commonly observed in a large number of cell types in response to stimulation by an extracellular agonist. In most cell types the mechanism of regular spiking is well understood and models based on Ca(2+)-induced Ca(2+) release (CICR) can account for many experimental observations. However, cells do not always exhibit simple Ca(2+) oscillations. In response to given agonists, some cells show more complex behaviour in the form of bursting, i.e. trains of Ca(2+) spikes separated by silent phases. Here we develop several theoretical models, based on physiologically plausible assumptions, that could account for complex intracellular Ca(2+) oscillations. The models are all based on one- or two-pool models based on CICR. We extend these models by (i) considering the inhibition of the Ca(2+)-release channel on a unique intracellular store at high cytosolic Ca(2+) concentrations, (ii) taking into account the Ca(2+)-activated degradation of inositol 1,4,5-trisphosphate (IP(3)), or (iii) considering explicity the evolution of the Ca(2+) concentration in two different pools, one sensitive and the other one insensitive to IP(3). Besides simple periodic oscillations, these three models can all account for more complex oscillatory behaviour in the form of bursting. Moreover, the model that takes the kinetics of IP(3) into account shows chaotic behaviour.

This model is hosted on BioModels Database and identifiedby: MODEL6622689184.

To cite BioModels Database, please use: BioModels Database: An enhanced, curated and annotated resourcefor published quantitative kinetic models.

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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 1

2.4 Unit area

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

Definition m²

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 three compartments.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
extracellular			3	1	litre		
cytosol			3	1	litre	$\overline{\mathbf{Z}}$	extracellular
intravesicular			3	1	litre	$ \overline{\mathbf{Z}} $	cytosol

3.1 Compartment extracellular

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

3.2 Compartment cytosol

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

3.3 Compartment intravesicular

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 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
					Condi- tion
			1 1–1		
EC		extracellular	μ mol·l ⁻¹	\Box	\Box
Z		cytosol	$\mu mol \cdot l^{-1}$	\Box	
Rho		cytosol	$\mu \text{mol} \cdot l^{-1}$		
Y		intravesicular	$\mu mol \cdot l^{-1}$		
Fraction-		cytosol	$\mu mol \cdot l^{-1}$	\Box	
$_{ m L}$ Inactive $_{ m L}$ Ch	annels				

5 Parameters

This model contains three global parameters.

Table 4: Properties of each parameter.

		*			
Id	Name	SBO	Value	Unit	Constant
a			40000.0		
d			100.0		\square
beta			1.0		

6 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 5: Overview of all reactions

N⁰	Id	Name	Reaction Equation	SBO
1	vin		$EC \longrightarrow Z$	
2	v2		$Z \longrightarrow Y$	
3	v3		$Y \xrightarrow{Rho} Z$	
4	v4		$Y \longrightarrow Z$	
5	v5		$Z \longrightarrow EC$	
6	v6		$Rho \xrightarrow{Z} Fraction_Inactive_Channels$	
7	v7		$Fraction_Inactive_Channels \longrightarrow Rho$	

6.1 Reaction vin

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

Reaction equation

$$EC \longrightarrow Z$$
 (1)

Reactant

Table 6: Properties of each reactant.

Id	Name	SBO
EC		

Product

Table 7: Properties of each product.

Id	Name	SBO
Z		

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \text{vol}(\text{cytosol}) \cdot (\text{v0} + \text{v1} \cdot \text{beta})$$
 (2)

Table 8: Properties of each parameter.

		1 1	
Id	Name	SBO Value Unit	Constant
ν0		1.0	\square
v1		1.0	

6.2 Reaction v2

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

Reaction equation

$$Z \longrightarrow Y$$
 (3)

Reactant

Table 9: Properties of each reactant.

Id	Name	SBO
Z		

Product

Table 10: Properties of each product.

Id	Name	SBO
Y		

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \text{vol}\left(\text{intravesicular}\right) \cdot \frac{\text{Vm2} \cdot [\mathbf{Z}]^2}{\text{K2}^2 + [\mathbf{Z}]^2}$$
 (4)

Table 11: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
Vm2		6.5	
K2		0.1	\square

6.3 Reaction v3

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

Reaction equation

$$Y \xrightarrow{\text{Rho}} Z$$
 (5)

Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
Y		

Modifier

Table 13: Properties of each modifier.

Id	Name	SBO
Rho	·	

Product

Table 14: Properties of each product.

Id	Name	SBO
Z		

Kinetic Law

Derived unit contains undeclared units

$$v_{3} = \text{vol}\left(\text{cytosol}\right) \cdot \frac{\text{beta} \cdot \frac{[\text{Rho}] \cdot \frac{a}{d} \cdot [Z]^{4}}{1 + \frac{a}{d} \cdot [Z]^{4}} \cdot \text{Vm3} \cdot [Y]^{2}}{\text{Ky}^{2} + [Y]^{2}}$$

$$\tag{6}$$

Table 15: Properties of each parameter.

		•			
Id	Name	SBO	Value	Unit	Constant
Vm3			50.0		lacksquare
Ку			0.2		$ \overline{\mathbf{Z}} $

6.4 Reaction v4

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

Reaction equation

$$Y \longrightarrow Z$$
 (7)

Reactant

Table 16: Properties of each reactant.

Id	Name	SBO
Y		

Product

Table 17: Properties of each product.

Id	Name	SBO
Z		

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \text{vol}(\text{cytosol}) \cdot \text{Kf} \cdot [Y] \tag{8}$$

Table 18: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
Kf		1.0	

6.5 Reaction v5

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

Reaction equation

$$Z \longrightarrow EC$$
 (9)

Reactant

Table 19: Properties of each reactant.

Id	Name	SBO
Z		

Product

Table 20: Properties of each product.

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \text{vol}\left(\text{extracellular}\right) \cdot \mathbf{K} \cdot [\mathbf{Z}]$$
 (10)

Table 21: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
K		10.0	

6.6 Reaction v6

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

Reaction equation

$$Rho \xrightarrow{Z} Fraction_Inactive_Channels$$
 (11)

Reactant

Table 22: Properties of each reactant.

Id	Name	SBO
Rho		

Modifier

Table 23: Properties of each modifier.

Id	Name	SBO
Z		

Product

Table 24: Properties of each product.

Id	Name	SBO
Fraction_Inactive_Channels		<u>. </u>

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \text{vol}(\text{cytosol}) \cdot \text{Kd} \cdot [\text{Z}]^4 \cdot [\text{Rho}]$$
 (12)

Table 25: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
Kd		5000.0	

6.7 Reaction v7

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

Reaction equation

Fraction_Inactive_Channels
$$\longrightarrow$$
 Rho (13)

Reactant

Table 26: Properties of each reactant.

Id	Name	SBO
Fraction_Inactive_Channels		

Product

Table 27: Properties of each product.

Id	Name	SBO
Rho		

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \text{vol}(\text{cytosol}) \cdot \text{Kr} \cdot (1 - [\text{Rho}]) \tag{14}$$

Table 28: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
Kr		5.0	

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.

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.

7.1 Species EC

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

This species takes part in two reactions (as a reactant in vin and as a product in v5).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{EC} = |v_5| - |v_1| \tag{15}$$

7.2 Species Z

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

This species takes part in six reactions (as a reactant in v2, v5 and as a product in vin, v3, v4 and as a modifier in v6).

$$\frac{\mathrm{d}}{\mathrm{d}t}Z = |v_1| + |v_3| + |v_4| - |v_2| - |v_5| \tag{16}$$

7.3 Species Rho

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

This species takes part in three reactions (as a reactant in v6 and as a product in v7 and as a modifier in v3).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Rho} = |v_7| - |v_6| \tag{17}$$

7.4 Species Y

Initial concentration $0.36 \ \mu mol \cdot l^{-1}$

This species takes part in three reactions (as a reactant in v3, v4 and as a product in v2).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{Y} = |v_2| - |v_3| - |v_4| \tag{18}$$

7.5 Species Fraction_Inactive_Channels

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

This species takes part in two reactions (as a reactant in v7 and as a product in v6).

$$\frac{d}{dt} Fraction_Inactive_Channels = v_6 - v_7$$
 (19)

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