SBML Model Report

Model name: "Meyer1991_CalciumSpike_ICC"

May 5, 2016

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by the following two authors: Vijayalakshmi Chelliah[1] and Philipp Bayer[2] at August fifth 2009 at 1:17 p. m. and last time modified at May 28th 2014 at 0:43 a. 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	2
species types	0	species	4
events	0	constraints	0
reactions	6	function definitions	0
global parameters	11	unit definitions	4
rules	0	initial assignments	0

Model Notes

This a model from the article:
Calcium spiking.
Meyer T, Stryer L Annu Rev Biophys Biophys Chem1991:20:153-74 1867714,

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Abstract:
No Abstract Available

The IP3-Ca2+ Crosscoupling Model (ICC) is reviewed by Meyer and Stryer in 1991, originally from Meyer and Stryer, 1988. PMID - 2455890 Parameters refer to figures 5 and 6 of the article which were reproduced by using Copasi 4.5 (Build 30).Species CaI and IP3 are buffered to 1% and 50% percent, respectively.

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To cite BioModels Database, please use Le Novre N., Bornstein B., Broicher A., Courtot M., Donizelli M., Dharuri H., Li L., Sauro H., Schilstra M., Shapiro B., Snoep J.L., Hucka M. (2006) BioModels Database: A Free, Centralized Database of Curated, Published, Quantitative Kinetic Models of Biochemical and Cellular Systems Nucleic Acids Res., 34: D689-D691.

2 Unit Definitions

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

2.1 Unit `microM`

Name microM

Definition $\mu\text{mol} \cdot \text{l}^{-1}$

2.2 Unit `microMpsec`

Name microMpsec

Definition $\mu\text{mol} \cdot \text{s}^{-1} \cdot \text{l}^{-1}$

2.3 Unit `microM4`

Name microM4

Definition $\mu\text{mol}^{-4} \cdot \text{s}^{-1} \cdot \text{l}^{-1}$

2.4 Unit `psec`

Name psec

Definition s^{-1}

2.5 Unit substance

Notes Mole is the predefined SBML unit for substance.

Definition mol

2.6 Unit volume

Notes Litre is the predefined SBML unit for volume.

Definition l

2.7 Unit area

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

Definition m^2

2.8 Unit length

Notes Metre is the predefined SBML unit for length since SBML Level 2 Version 1.

Definition m

2.9 Unit time

Notes Second is the predefined SBML unit for time.

Definition s

3 Compartments

This model contains two compartments.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
cytosol		0000290	3	1	litre	☑	
ER_store		0000290	3	1	litre	☑	cytosol

3.1 Compartment cytosol

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

SBO:0000290 physical compartment

3.2 Compartment ER_store

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

SBO:0000290 physical compartment

4 Species

This model contains four 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
CaI		cytosol	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
IP3		cytosol	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
CaS		ER_store	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
g		cytosol	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟

5 Parameters

This model contains eleven global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
A			20.00	s^{-1}	☑
B			40.00	$\mu mol \cdot s^{-1} \cdot l^{-1}$	☑
C			1.10	$\mu mol \cdot s^{-1} \cdot l^{-1}$	☑
D			2.00	s^{-1}	☑
E			1.00	$\mu mol^{-4} \cdot s^{-1} \cdot l^{-1}$	☑
F			0.02	s^{-1}	☑
k1			0.50	$\mu mol \cdot l^{-1}$	☑
k2			0.15	$\mu mol \cdot l^{-1}$	☑
k3			1.00	$\mu mol \cdot l^{-1}$	☑
L			0.01	s^{-1}	☑
R			0.09		☑

6 Reactions

This model contains six 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	JChannel		$\mathrm{CaS} \xrightarrow{\mathrm{IP3,\ g}} \mathrm{CaI}$	
2	JPump		$\mathrm{CaI} \longrightarrow \mathrm{CaS}$	
3	kPLC		$\emptyset \xrightarrow{\mathrm{CaI}} \mathrm{IP3}$	
4	kPhosphatase		$\mathrm{IP3} \longrightarrow \emptyset$	
5	inhibition_parameter1		$\emptyset \xrightarrow{\mathrm{CaI}} \mathrm{g}$	
6	inhibition_parameter2		$\mathrm{g} \xrightarrow{\mathrm{CaI}} \emptyset$	

6.1 Reaction JChannel

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

Reaction equation

$$\mathrm{CaS} \xrightarrow{\mathrm{IP3,\ g}} \mathrm{CaI} \tag{1}$$

Reactant

Table 6: Properties of each reactant.

Id	Name	SBO
CaS		

Modifiers

Table 7: Properties of each modifier.

Id	Name	SBO
IP3		
g		

Product

Table 8: Properties of each product.

Id	Name	SBO
CaI		

Kinetic Law

Derived unit contains undeclared units

$$v_1 = (1 - [\mathrm{g}]) \cdot \left(\frac{\mathrm{A} \cdot ([\mathrm{IP3}] \cdot 0.5)^4}{([\mathrm{IP3}] \cdot 0.5 + \mathrm{k1})^4} + \mathrm{L} \right) \cdot [\mathrm{CaS}] \tag{2}$$

6.2 Reaction JPump

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

Reaction equation

$$\mathrm{CaI} \longrightarrow \mathrm{CaS} \tag{3}$$

Reactant

Table 9: Properties of each reactant.

Id	Name	SBO
CaI		

Product

Table 10: Properties of each product.

Id	Name	SBO
CaS		

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \frac{\mathrm{B} \cdot (\mathrm{[CaI]} \cdot 0.01)^2}{(\mathrm{[CaI]} \cdot 0.01)^2 + \mathrm{k2}^2} \tag{4}$$

6.3 Reaction kPLC

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

Reaction equation

$$\emptyset \xrightarrow{\mathrm{CaI}} \mathrm{IP3} \tag{5}$$

Modifier

Table 11: Properties of each modifier.

Id	Name	SBO
CaI		

Product

Table 12: Properties of each product.

Id	Name	SBO
IP3		

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \mathrm{C} \cdot \left(1 - \frac{\mathrm{k3}}{[\mathrm{CaI}] \cdot 0.01 + \mathrm{k3}} \cdot \frac{1}{1 + \mathrm{R}}\right) \tag{6}$$

6.4 Reaction kPhosphatase

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

Reaction equation

$$\mathrm{IP3} \longrightarrow \emptyset \tag{7}$$

Reactant

Table 13: Properties of each reactant.

Id	Name	SBO
IP3		

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \mathrm{D} \cdot [\mathrm{IP3}] \cdot 0.5 \tag{8}$$

6.5 Reaction inhibition_parameter1

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

Reaction equation

$$\emptyset \xrightarrow{\mathrm{CaI}} \mathrm{g} \tag{9}$$

Modifier

Table 14: Properties of each modifier.

Id	Name	SBO
CaI		

Product

Table 15: Properties of each product.

Id	Name	SBO
g		

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \mathrm{E} \cdot ([\mathrm{CaI}] \cdot 0.01)^4 \cdot (1 - [\mathrm{g}]) \tag{10}$$

6.6 Reaction inhibition_parameter2

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

Reaction equation

$$\mathrm{g} \xrightarrow{\mathrm{CaI}} \emptyset \tag{11}$$

Reactant

Table 16: Properties of each reactant.

Id	Name	SBO
g		

Modifier

Table 17: Properties of each modifier.

Id	Name	SBO
CaI		

Kinetic Law

Derived unit s^{-1}

$$v_6 = \mathrm{F} \tag{12}$$

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 `CaI`

SBO:0000247 simple chemical

Initial concentration $0.1\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in five reactions (as a reactant in `JPump` and as a product in `JChannel` and as a modifier in `kPLC`, `inhibition_parameter1`, `inhibition_parameter2`).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{CaI} = v_1 - v_2 \tag{13}$$

7.2 Species `IP3`

SBO:0000247 simple chemical

Initial concentration $0.05\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in three reactions (as a reactant in `kPhosphatase` and as a product in `kPLC` and as a modifier in `JChannel`).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{IP3} = v_3 - v_4 \tag{14}$$

7.3 Species CaS

SBO:0000247 simple chemical

Initial concentration $1100\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in JChannel and as a product in JPump).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{CaS} = v_2 - v_1 \tag{15}$$

7.4 Species g

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

This species takes part in three reactions (as a reactant in inhibition_parameter2 and as a product in inhibition_parameter1 and as a modifier in JChannel).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{g} = v_5 - v_6 \tag{16}$$

A Glossary of Systems Biology Ontology Terms

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

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

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