SBML Model Report

Model name: "Goldbeter1990_CalciumSpike_CICR"

May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 1 format. This model was created by Harish Dharuri[1] at March 21st 2007 at 3:41 p. m. and last time modified at May 24th 2014 at 5:41 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	2
species types	0	species	2
events	0	constraints	0
reactions	6	function definitions	0
global parameters	13	unit definitions	4
rules	0	initial assignments	0

Model Notes

The model reproduces the time profile of cytosolic and intracellular calcium as depicted in the upper panel of Fig 2 in the paper. The model was successfully tested on MathSBML and Jarnac.

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[1] California Institute of Technology, hdharuri@cds.caltech.edu

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 eight unit definitions of which four are predefined by SBML and not mentioned in the model.

2.1 Unit `substance`

Name micromole

Definition µmol

2.2 Unit `uM_per_sec`

Name uM_per_sec

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

2.3 Unit `sec_inv`

Name sec_inv

Definition s^{-1}

2.4 Unit `uM`

Name uM

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

2.5 Unit `volume`

Notes Litre is the predefined SBML unit for `volume`.

Definition l

2.6 Unit `area`

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

Definition m^2

2.7 Unit `length`

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

Definition m

2.8 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`	cytosol		3	1	litre	☑	
`store`	store		3	1	litre	☑	

3.1 Compartment `cytosol`

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

Name cytosol

3.2 Compartment `store`

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

Name store

4 Species

This model contains two 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
Z		cytosol	$\mu mol \cdot l^{-1}$	⊟	⊟
Y		store	$\mu mol \cdot l^{-1}$	⊟	⊟

5 Parameters

This model contains 13 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
v0			1.000	$\mu mol \cdot l^{-1} \cdot s^{-1}$	☑
v1			7.300	$\mu mol \cdot l^{-1} \cdot s^{-1}$	☑
beta			0.301	dimensionless	☑
Vm2			65.000	$\mu mol \cdot l^{-1} \cdot s^{-1}$	☑
n			2.000	dimensionless	☑
K2			1.000	$\mu mol \cdot l^{-1}$	☑
Vm3			500.000	$\mu mol \cdot l^{-1} \cdot s^{-1}$	☑
m			2.000	dimensionless	☑
Kr			2.000	$\mu mol \cdot l^{-1}$	☑
Ka			0.900	$\mu mol \cdot l^{-1}$	☑
kf			1.000	s^{-1}	☑
k			10.000	s^{-1}	☑
p			4.000	dimensionless	☑

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	R0	Ca influx	$\emptyset \longrightarrow Z$	
2	R1	InsP3 dependent Ca influx	$\emptyset \longrightarrow Z$	
3	R2	ATP driven Ca pumping into store	$Z \longrightarrow Y$	
4	R3	ATP driven pumping into cytosol	$Y \longrightarrow Z$	
5	Rf	Ca leak	$Y \longrightarrow Z$	
6	R_eff	Ca efflux	$Z \longrightarrow \emptyset$	

6.1 Reaction R0

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

Name Ca influx

Reaction equation

$$\emptyset \longrightarrow \mathrm{Z} \tag{1}$$

Product

Table 6: Properties of each product.

Id	Name	SBO
Z		

Kinetic Law

Derived unit $\mu\mathrm{mol} \cdot \mathrm{s}^{-1}$

$$v_1 = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{v0} \tag{2}$$

6.2 Reaction R1

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

Name InsP3 dependent Ca influx

Reaction equation

$$\emptyset \longrightarrow \mathrm{Z} \tag{3}$$

Product

Table 7: Properties of each product.

Id	Name	SBO
Z		

Kinetic Law

Derived unit $\mu\mathrm{mol} \cdot \mathrm{s}^{-1}$

$$v_2 = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{v1} \cdot \mathrm{beta} \tag{4}$$

6.3 Reaction R2

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

Name ATP driven Ca pumping into store

Reaction equation

$$\mathrm{Z} \longrightarrow \mathrm{Y} \tag{5}$$

Reactant

Table 8: Properties of each reactant.

Id	Name	SBO
Z		

Product

Table 9: Properties of each product.

Id	Name	SBO
Y		

Kinetic Law

Derived unit $1.0000000000000024 \cdot 10^{-6}\ \mathrm{mol} \cdot \mathrm{s}^{-1}$

$$v_3 = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \frac{\mathrm{Vm2} \cdot [\mathrm{Z}]^{\mathrm{n}}}{\mathrm{K2}^{\mathrm{n}} + [\mathrm{Z}]^{\mathrm{n}}} \tag{6}$$

6.4 Reaction R3

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

Name ATP driven pumping into cytosol

Reaction equation

$$\mathrm{Y} \longrightarrow \mathrm{Z} \tag{7}$$

Reactant

Table 10: Properties of each reactant.

Id	Name	SBO
Y		

Product

Table 11: Properties of each product.

Id	Name	SBO
Z		

Kinetic Law

Derived unit $1.0000000000000022 \cdot 10^{-6}\ \mathrm{mol} \cdot \mathrm{s}^{-1}$

$$v_4 = \mathrm{vol}\,(\mathrm{store}) \cdot \frac{\mathrm{Vm3} \cdot [\mathrm{Y}]^{\mathrm{m}} \cdot [\mathrm{Z}]^{\mathrm{p}}}{(\mathrm{Kr}^{\mathrm{m}} + [\mathrm{Y}]^{\mathrm{m}}) \cdot (\mathrm{Ka}^{\mathrm{p}} + [\mathrm{Z}]^{\mathrm{p}})} \tag{8}$$

6.5 Reaction Rf

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

Name Ca leak

Reaction equation

$$\mathrm{Y} \longrightarrow \mathrm{Z} \tag{9}$$

Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
Y		

Product

Table 13: Properties of each product.

Id	Name	SBO
Z		

Id	Name	SBO

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot \mu\mathrm{mol}$

$$v_5 = \mathrm{vol}\,(\mathrm{store}) \cdot \mathrm{kf} \cdot [\mathrm{Y}] \tag{10}$$

6.6 Reaction R_eff

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

Name Ca efflux

Reaction equation

$$\mathrm{Z} \longrightarrow \emptyset \tag{11}$$

Reactant

Table 14: Properties of each reactant.

Id	Name	SBO
Z		

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot \mu\mathrm{mol}$

$$v_6 = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{k} \cdot [\mathrm{Z}] \tag{12}$$

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.

7.1 Species Z

Initial concentration $0.15\ \mu\mathrm{mol} \cdot \mathrm{l}^{-1}$

This species takes part in six reactions (as a reactant in R2, R_eff and as a product in R0, R1, R3, Rf).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Z} = v_1 + v_2 + v_4 + v_5 - v_3 - v_6 \tag{13}$$

7.2 Species Y

Initial concentration $1.6\ \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in three reactions (as a reactant in R3, Rf and as a product in R2).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Y} = v_3 - v_4 - v_5 \tag{14}$$

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