SBML Model Report

Model name: “Wang2007 - ATP induced intracellular Calcium Oscillation”

May 5, 2016

1 General Overview

This is a document in SBML Level 2 Version 1 format. This model was created by the following two authors: Harish Dharuri[1] and Vijayalakshmi Chelliah[2] at August 28th 2007 at 2:35 p. m. and last time modified at March 31st 2014 at 11:58 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	7
events	0	constraints	0
reactions	11	function definitions	0
global parameters	32	unit definitions	1
rules	10	initial assignments	0

Model Notes

Wang2007 - ATP induced intracellular Calicum Oscillation

The model simulate the ATP-induced intracellular Ca^{2+} oscillations and the quantitative effect of ATP concentration on the oscillation characteristics such as the duration, peak concentration of intracellular Ca^{2+} and average interval.

[1]California Institute of Technology, hdharuri@cds.caltech.edu
[2]EMBL-EBI, viji@ebi.ac.uk

This model is described in the article:A quantitative kinetic model for ATP-induced intracellular Ca2+ oscillations.Wang J, Huang X, Huang W.J. Theor. Biol. 2007 Apr; 245(3): 510-519

Abstract:

A quantitative kinetic model is proposed to simulate the ATP-induced intracellular Ca(2+) oscillations. The quantitative effect of ATP concentration upon the oscillations was successfully simulated. Our simulation results support previous experimental explanations that the Ca(2+) oscillations are mainly due to interaction of Ca(2+) release from the endoplasmic reticulum (ER) and the ATP-dependent Ca(2+) pump back into the ER, and the oscillations are prolonged by extracellular Ca(2+) entry that maintains the constant Ca(2+) supplies to its intracellular stores. The model is also able to simulate the sudden disappearance phenomenon of the Ca(2+) oscillations observed in some cell types by taking into account of the biphasic characteristic of the Ca(2+) release from the endoplasmic reticulum (ER). Moreover, the model simulation results for the Ca(2+) oscillations characteristics such as duration, peak [Ca(2+)](cyt), and average interval, etc., lead to prediction of some possible factors responsible for the variations of Ca(2+) oscillations in different types of cells.

This model is hosted on BioModels Database and identifiedby: BIOMD0000000145.

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

2 Unit Definitions

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

2.1 Unit `substance`

Name nano mole

Definition nmol

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 two compartments.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
Cytosol			3	1	litre	☑	
ER			3	1	litre	☑	

3.1 Compartment Cytosol

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.

4 Species

This model contains seven 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
Galpha_GTP	Galpha_GTP	Cytosol	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
APLC	APLC	Cytosol	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
IP3	IP3	Cytosol	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Ca_ER	Calcium	ER	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Ca_Cyt	Calcium	Cytosol	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
PLC	PLC	Cytosol	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
DG	Diacylglycerol	Cytosol	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟

5 Parameters

This model contains 32 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Raplc			0.00		☐
Kp			4.00		☑
Rpkc			0.00		☐
Kd			10.00		☑
Kr			200.00		☑
Rgalpha_gtp			0.00		☐
n			4.00		☑
Kg			25.00		☑
Rdg			0.00		☐
m			2.00		☑
Rip3			0.00		☐
Ks			25.00		☑
Rcyt1			0.00		☐
Kc1			1000.00		☑
Rcyt2			0.00		☐
Kc2			2000.00		☑
Rer			0.00		☐
w			3.00		☑
Ker			75.00		☑
Cplc_total			10.00		☑
k0			0.10		☑
k1			3.40		☑
k2			4.00		☑
k3			4.50		☑
k4			1.20		☑
k5			0.12		☑
k6			14.00		☑
k7			2.00		☑
k8			10500.00		☑
k9			600.00		☑
k10			3000.00		☑
k11			260.00		☑

6 Rules

This is an overview of ten rules.

6.1 Rule DG

Rule DG is an assignment rule for species DG:

$$\mathrm{DG} = [\mathrm{IP3}] \tag{1}$$

Derived unit $\mathrm{nmol} \cdot \mathrm{l}^{-1}$

6.2 Rule Raplc

Rule Raplc is an assignment rule for parameter Raplc:

$$\mathrm{Raplc} = \frac{[\mathrm{APLC}]}{\mathrm{Kp} + [\mathrm{APLC}]} \tag{2}$$

6.3 Rule Rpkc

Rule Rpkc is an assignment rule for parameter Rpkc:

$$\mathrm{Rpkc} = \frac{\frac{[\mathrm{DG}]}{\mathrm{Kd}+[\mathrm{DG}]} \cdot [\mathrm{Ca\_Cyt}]}{\mathrm{Kr} + [\mathrm{Ca\_Cyt}]} \tag{3}$$

6.4 Rule Rgalpha_gtp

Rule Rgalpha_gtp is an assignment rule for parameter Rgalpha_gtp:

$$\mathrm{Rgalpha\_gtp} = \frac{[\mathrm{Galpha\_GTP}]^{\mathrm{n}}}{\mathrm{Kg}^{\mathrm{n}} + [\mathrm{Galpha\_GTP}]^{\mathrm{n}}} \tag{4}$$

6.5 Rule Rdg

Rule Rdg is an assignment rule for parameter Rdg:

$$\mathrm{Rdg} = \frac{[\mathrm{DG}]^{\mathrm{m}}}{\mathrm{Kd}^{\mathrm{m}} + [\mathrm{DG}]^{\mathrm{m}}} \tag{5}$$

6.6 Rule Rip3

Rule Rip3 is an assignment rule for parameter Rip3:

$$\mathrm{Rip3} = \frac{[\mathrm{IP3}]^3}{\mathrm{Ks}^3 + [\mathrm{IP3}]^3} \tag{6}$$

6.7 Rule `Rcyt1`

Rule `Rcyt1` is an assignment rule for parameter `Rcyt1`:

$$\mathrm{Rcyt1} = \frac{[\mathrm{Ca\_Cyt}]}{\mathrm{Kc1} + [\mathrm{Ca\_Cyt}]} \tag{7}$$

6.8 Rule `Rcyt2`

Rule `Rcyt2` is an assignment rule for parameter `Rcyt2`:

$$\mathrm{Rcyt2} = \frac{[\mathrm{Ca\_Cyt}]}{\mathrm{Kc2} + [\mathrm{Ca\_Cyt}]} \tag{8}$$

6.9 Rule `Rer`

Rule `Rer` is an assignment rule for parameter `Rer`:

$$\mathrm{Rer} = \frac{[\mathrm{Ca\_ER}]^{\mathrm{w}}}{\mathrm{Ker}^{\mathrm{w}} + [\mathrm{Ca\_ER}]^{\mathrm{w}}} \tag{9}$$

6.10 Rule `PLC`

Rule `PLC` is an assignment rule for species `PLC`:

$$\mathrm{PLC} = \mathrm{Cplc\_total} - [\mathrm{APLC}] \tag{10}$$

7 Reactions

This model contains eleven 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	R1		$\emptyset \longrightarrow$ Galpha_GTP	
2	R2		$\emptyset \longrightarrow$ Galpha_GTP	
3	R3		Galpha_GTP $\longrightarrow \emptyset$	
4	R4		Galpha_GTP $\longrightarrow \emptyset$	
5	R5		$\emptyset \xrightarrow{\text{PLC}}$ APLC	
6	R6		APLC $\longrightarrow \emptyset$	
7	R7		$\emptyset \xrightarrow{\text{APLC}}$ IP3	
8	R8		IP3 $\longrightarrow \emptyset$	
9	R9		$0 \cdot 0010$ Ca_ER $\rightleftharpoons 0 \cdot 01$ Ca_Cyt	
10	R10		$0 \cdot 05$ Ca_Cyt $\longrightarrow \emptyset$	
11	R11		$\emptyset \longrightarrow 0 \cdot 05$ Ca_Cyt	

7.1 Reaction R1

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

Reaction equation

$$\emptyset \longrightarrow \text{Galpha\_GTP} \tag{11}$$

Product

Table 6: Properties of each product.

Id	Name	SBO
Galpha_GTP	Galpha_GTP	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \text{vol}\,(\text{Cytosol}) \cdot \text{k0} \tag{12}$$

7.2 Reaction R2

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

Reaction equation

$$\emptyset \longrightarrow \text{Galpha\_GTP} \tag{13}$$

Product

Table 7: Properties of each product.

Id	Name	SBO
Galpha_GTP	Galpha_GTP	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \text{vol}\,(\text{Cytosol}) \cdot \text{k1} \cdot [\text{Galpha\_GTP}] \tag{14}$$

7.3 Reaction R3

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

Reaction equation

$$\text{Galpha\_GTP} \longrightarrow \emptyset \tag{15}$$

Reactant

Table 8: Properties of each reactant.

Id	Name	SBO
Galpha_GTP	Galpha_GTP	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \text{vol}\,(\text{Cytosol}) \cdot \text{k2} \cdot \text{Raplc} \cdot [\text{Galpha\_GTP}] \tag{16}$$

7.4 Reaction R4

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

Reaction equation

$$\text{Galpha\_GTP} \longrightarrow \emptyset \tag{17}$$

Reactant

Table 9: Properties of each reactant.

Id	Name	SBO
Galpha_GTP	Galpha_GTP	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \text{vol}\,(\text{Cytosol}) \cdot \text{k3} \cdot \text{Rpkc} \cdot [\text{Galpha\_GTP}] \tag{18}$$

7.5 Reaction R5

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

Reaction equation

$$\emptyset \xrightarrow{\text{PLC}} \text{APLC} \tag{19}$$

Modifier

Table 10: Properties of each modifier.

Id	Name	SBO
PLC	PLC	

Product

Table 11: Properties of each product.

Id	Name	SBO
APLC	APLC	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \text{vol}\,(\text{Cytosol}) \cdot \text{k4} \cdot \text{Rgalpha\_gtp} \cdot \text{Rdg} \cdot [\text{PLC}] \tag{20}$$

7.6 Reaction R6

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

Reaction equation

$$\text{APLC} \longrightarrow \emptyset \tag{21}$$

Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
APLC	APLC	

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \mathrm{vol}\,(\mathrm{Cytosol}) \cdot \mathrm{k5} \cdot [\mathrm{APLC}] \tag{22}$$

7.7 Reaction R7

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

Reaction equation

$$\emptyset \xrightarrow{\mathrm{APLC}} \mathrm{IP3} \tag{23}$$

Modifier

Table 13: Properties of each modifier.

Id	Name	SBO
APLC	APLC	

Product

Table 14: Properties of each product.

Id	Name	SBO
IP3	IP3	

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \mathrm{vol}\,(\mathrm{Cytosol}) \cdot \mathrm{k6} \cdot [\mathrm{APLC}] \tag{24}$$

7.8 Reaction R8

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

Reaction equation

$$\mathrm{IP3} \longrightarrow \emptyset \tag{25}$$

Reactant

Table 15: Properties of each reactant.

Id	Name	SBO
IP3	IP3	

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \mathrm{vol}\,(\mathrm{Cytosol}) \cdot \mathrm{k7} \cdot [\mathrm{IP3}] \tag{26}$$

7.9 Reaction R9

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

Reaction equation

$$0{\cdot}0010\,\mathrm{Ca\_ER} \rightleftharpoons 0{\cdot}01\,\mathrm{Ca\_Cyt} \tag{27}$$

Reactant

Table 16: Properties of each reactant.

Id	Name	SBO
Ca_ER	Calcium	

Product

Table 17: Properties of each product.

Id	Name	SBO
Ca_Cyt	Calcium	

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \mathrm{vol}\,(\mathrm{ER}) \cdot (\mathrm{k8} \cdot \mathrm{Rip3} \cdot \mathrm{Rer} - \mathrm{k9} \cdot \mathrm{Rcyt1}) \tag{28}$$

7.10 Reaction R10

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

Reaction equation

$$0{\cdot}05\,\mathrm{Ca\_Cyt} \longrightarrow \emptyset \tag{29}$$

Reactant

Table 18: Properties of each reactant.

Id	Name	SBO
Ca_Cyt	Calcium	

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = \mathrm{vol}\,(\mathrm{Cytosol}) \cdot \mathrm{k10} \cdot \mathrm{Rcyt2} \tag{30}$$

7.11 Reaction R11

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

Reaction equation

$$\emptyset \longrightarrow 0{\cdot}05\,\mathrm{Ca\_Cyt} \tag{31}$$

Product

Table 19: Properties of each product.

Id	Name	SBO
Ca_Cyt	Calcium	

Kinetic Law

Derived unit contains undeclared units

$$v_{11} = \mathrm{vol}\,(\mathrm{Cytosol}) \cdot \mathrm{k11} \tag{32}$$

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 Galpha_GTP

Name Galpha_GTP

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

This species takes part in four reactions (as a reactant in R3, R4 and as a product in R1, R2).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Galpha\_GTP} = v_1 + v_2 - v_3 - v_4 \tag{33}$$

8.2 Species APLC

Name APLC

Initial concentration $9\ \mathrm{nmol} \cdot \mathrm{l}^{-1}$

This species takes part in three reactions (as a reactant in R6 and as a product in R5 and as a modifier in R7).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{APLC} = v_5 - v_6 \tag{34}$$

8.3 Species IP3

Name IP3

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

This species takes part in two reactions (as a reactant in R8 and as a product in R7).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{IP3} = v_7 - v_8 \tag{35}$$

8.4 Species Ca_ER

Name Calcium

Initial concentration $1000\ \mathrm{nmol} \cdot \mathrm{l}^{-1}$

This species takes part in one reaction (as a reactant in R9).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Ca\_ER} = -0.0010\, v_9 \tag{36}$$

8.5 Species Ca_Cyt

Name Calcium

Initial concentration $200\ \mathrm{nmol} \cdot \mathrm{l}^{-1}$

This species takes part in three reactions (as a reactant in R10 and as a product in R9, R11).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Ca\_Cyt} = 0.01\ v_9 + 0.05\ v_{11} - 0.05\ v_{10} \tag{37}$$

8.6 Species PLC

Name PLC

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

Involved in rule PLC

This species takes part in one reaction (as a modifier in R5) and is also involved in one rule which determines this species' quantity.

8.7 Species DG

Name Diacylglycerol

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

Involved in rule DG

One rule which determines this species' quantity.

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