SBML Model Report

Model name: "Lavrentovich2008_Ca_Oscillations"

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1 General Overview

This is a document in SBML Level 2 Version 3 format. This model was created by the following two authors: Harish Dharuri[1] and Lukas Endler[2] at August 21st 2008 at 11:36 a. m. and last time modified at July eleventh 2012 at 5:45 p. 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	2
species types	0	species	3
events	0	constraints	0
reactions	7	function definitions	0
global parameters	14	unit definitions	4
rules	0	initial assignments	0

Model Notes

The model reproduces the time profile of cytoplasmic Calcium as depicted in Fig 3 of the paper. Model successfully reproduced using Jarnac and MathSBML.

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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 micro mole

Definition $\mu\mathrm{mol}$

2.2 Unit `uM`

Name uM

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

2.3 Unit `uM_sec_1`

Name uM_sec_1

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

2.4 Unit `sec_1`

Name sec_1

Definition s^{-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
compartment	Cytoplasm		3	1	litre	☑	
ER	Endoplasmic Reticulum		3	1	litre	☑	

3.1 Compartment compartment

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

Name Cytoplasm

3.2 Compartment ER

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

Name Endoplasmic Reticulum

4 Species

This model contains three 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
X	Cytoplasmic Calcium	compartment	$\mu mol \cdot l^{-1}$	⊟	⊟
Y	Calcium in ER	ER	$\mu mol \cdot l^{-1}$	⊟	⊟
Z	IP3	compartment	$\mu mol \cdot l^{-1}$	⊟	⊟

5 Parameters

This model contains 14 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
vin			0.05	$\mu mol \cdot l^{-1} \cdot s^{-1}$	☑
kout			0.50	s^{-1}	☑
vM3			40.00	s^{-1}	☑
k_CaA			0.15	$\mu mol \cdot l^{-1}$	☑
n			2.02	dimensionless	☑
k_CaI			0.15	$\mu mol \cdot l^{-1}$	☑
m			2.20	dimensionless	☑
kip3			0.10	$\mu mol \cdot l^{-1}$	☑
vM2			15.00	$\mu mol \cdot l^{-1} \cdot s^{-1}$	☑
k2			0.10	$\mu mol \cdot l^{-1}$	☑
kf			0.50	s^{-1}	☑
vp			0.05	$\mu mol \cdot l^{-1} \cdot s^{-1}$	☑
kp			0.30	$\mu mol \cdot l^{-1}$	☑
kdeg			0.08	s^{-1}	☑

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

№	Id	Name	Reaction Equation	SBO
1	R1	vin	$\emptyset \longrightarrow X$	
2	R2	Calcium export from cell	$X \longrightarrow \emptyset$	
3	R3	CICR	$Y \xrightarrow{Z} X$	
4	R4	serca	$X \longrightarrow Y$	
5	R5	Leak flux	$Y \longrightarrow X$	
6	R6	PLC	$\emptyset \xrightarrow{X} Z$	
7	R7	IP3 degradation	$Z \longrightarrow \emptyset$	

6.1 Reaction R1

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

Name vin

Reaction equation

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

Product

Table 6: Properties of each product.

Id	Name	SBO
X	Cytoplasmic Calcium	

Kinetic Law

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

$$v_1 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{vin} \tag{2}$$

6.2 Reaction R2

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

Name Calcium export from cell

Reaction equation

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

Reactant

Table 7: Properties of each reactant.

Id	Name	SBO
X	Cytoplasmic Calcium	

Kinetic Law

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

$$v_2 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{kout} \cdot [\mathrm{X}] \tag{4}$$

6.3 Reaction R3

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

Name CICR

Reaction equation

$$\mathrm{Y} \xrightarrow{\mathrm{Z}} \mathrm{X} \tag{5}$$

Reactant

Table 8: Properties of each reactant.

Id	Name	SBO
Y	Calcium in ER	

Modifier

Table 9: Properties of each modifier.

Id	Name	SBO
Z	IP3	

Product

Table 10: Properties of each product.

Id	Name	SBO
X	Cytoplasmic Calcium	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \mathrm{vol}\,(\mathrm{ER}) \cdot 4 \cdot \mathrm{vM3} \cdot \mathrm{k\_CaA}^{\mathrm{n}} \cdot \frac{[\mathrm{X}]^{\mathrm{n}}}{([\mathrm{X}]^{\mathrm{n}} + \mathrm{k\_CaA}^{\mathrm{n}}) \cdot ([\mathrm{X}]^{\mathrm{n}} + \mathrm{k\_CaI}^{\mathrm{n}})} \cdot \frac{[\mathrm{Z}]^{\mathrm{m}}}{[\mathrm{Z}]^{\mathrm{m}} + \mathrm{kip3}^{\mathrm{m}}} \cdot ([\mathrm{Y}] - [\mathrm{X}]) \tag{6}$$

6.4 Reaction R4

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

Name serca

Reaction equation

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

Reactant

Table 11: Properties of each reactant.

Id	Name	SBO
X	Cytoplasmic Calcium	

Product

Table 12: Properties of each product.

Id	Name	SBO
Y	Calcium in ER	

Kinetic Law

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

$$v_4 = \frac{\mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{vM2} \cdot [\mathrm{X}]^2}{[\mathrm{X}]^2 + \mathrm{k2}^2} \tag{8}$$

6.5 Reaction R5

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

Name Leak flux

Reaction equation

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

Reactant

Table 13: Properties of each reactant.

Id	Name	SBO
Y	Calcium in ER	

Product

Table 14: Properties of each product.

Id	Name	SBO
X	Cytoplasmic Calcium	

Kinetic Law

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

$$v_5 = \mathrm{vol}(\mathrm{ER}) \cdot \mathrm{kf} \cdot ([\mathrm{Y}] - [\mathrm{X}]) \tag{10}$$

6.6 Reaction R6

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

Name PLC

Reaction equation

$$\emptyset \xrightarrow{\mathrm{X}} \mathrm{Z} \tag{11}$$

Modifier

Table 15: Properties of each modifier.

Id	Name	SBO
X	Cytoplasmic Calcium	

Product

Table 16: Properties of each product.

Id	Name	SBO
Z	IP3	

Kinetic Law

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

$$v_6 = \frac{\mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{vp} \cdot [\mathrm{X}]^2}{[\mathrm{X}]^2 + \mathrm{kp}^2} \tag{12}$$

6.7 Reaction R7

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

Name IP3 degradation

Reaction equation

$$\mathrm{Z} \longrightarrow \emptyset \tag{13}$$

Reactant

Table 17: Properties of each reactant.

Id	Name	SBO
Z	IP3	

Kinetic Law

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

$$v_7 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{kdeg} \cdot [\mathrm{Z}] \tag{14}$$

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 X

Name Cytoplasmic Calcium

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

This species takes part in six reactions (as a reactant in R2, R4 and as a product in R1, R3, R5 and as a modifier in R6).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{X} = v_1 + v_3 + v_5 - v_2 - v_4 \tag{15}$$

7.2 Species Y

Name Calcium in ER

Initial concentration $1.5\ \mu\text{mol}\cdot\text{l}^{-1}$

This species takes part in three reactions (as a reactant in R3, R5 and as a product in R4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Y} = v_4 - v_3 - v_5 \tag{16}$$

7.3 Species Z

Name IP3

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

This species takes part in three reactions (as a reactant in R7 and as a product in R6 and as a modifier in R3).

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

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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