SBML Model Report

Model name: "ChenXF2008_CICR"



May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 3 format. This model was created by Harish Dharuri¹ at November 24th 2008 at 7:12 a.m. and last time modified at February 24th 2015 at 8:33 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	3
species types	0	species	9
events	0	constraints	0
reactions	15	function definitions	0
global parameters	38	unit definitions	5
rules	3	initial assignments	0

Model Notes

The model reproduces the plots in Figures 1 and 2. Note that the units of the time scale "A, are not right in the paper, it was corrected by the curator. Model successfully tested on MathSBML.

2 Unit Definitions

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

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2.1 Unit substance

Name micromole

Definition µmol

2.2 Unit uM

Name uM

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

2.3 Unit s_1

Name s_1

Definition s^{-1}

2.4 Unit uM_s_1

Name uM_s_1

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

2.5 Unit uM_1_s_1

Name $uM_1_s_1$

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

2.6 Unit volume

Notes Litre is the predefined SBML unit for volume.

Definition 1

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 three compartments.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
Cytoplasm			3	1	litre		
ER			3	0.185	1		
PM			3	1	litre		

3.1 Compartment Cytoplasm

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 0.185 litre.

3.3 Compartment PM

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

Produced by SBML2ATEX

4 Species

This model contains nine 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 Condi- tion
Ca_Cyt		Cytoplasm	μ mol·l ⁻¹	⊣	\Box
IP3_Cyt		Cytoplasm	$\mu mol \cdot l^{-1}$		
Ca_ER		ER	$\mu mol \cdot l^{-1}$		
S2		ER	μ mol·l ⁻¹		
S2a		ER	μ mol·l ⁻¹		
S4		ER	$\mu mol \cdot l^{-1}$		
Ос		PM	$\mu mol \cdot l^{-1}$		
0_0		PM	$\mu mol \cdot l^{-1}$		
Orai1		PM	$\mu mol \cdot l^{-1}$		

5 Parameters

This model contains 38 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
L			$9.3 \cdot 10^{-4}$	s^{-1}	
$P_{-}IP3R$			66.600	s^{-1}	$\overline{\mathbf{Z}}$
Ki			1.000	μ mol·l ⁻¹	$\overline{\mathbf{Z}}$
$k_{-}i$			6.000	s^{-1}	$\overline{\mathbf{Z}}$
Ka			0.400	μ mol·l ⁻¹	$\overline{\mathbf{Z}}$
V_SERCA			1.000	$\mu mol \cdot l^{-1} \cdot s^{-1}$	$\overline{\mathbf{Z}}$
p			2.000	dimensionless	$\overline{\mathbf{Z}}$
K_SERCA			0.150	$\mu mol \cdot l^{-1}$	$\overline{\mathbf{Z}}$
k_soc			2.300	$\mu \text{mol}^{-1} \cdot 1 \cdot \text{s}^{-1}$	$\overline{\mathbf{Z}}$
V_PMleak			$5 \cdot 10^{-7}$	s^{-1}	\overline{Z}
Ca_ec			1500.000	μ mol·l ⁻¹	\overline{Z}
V_PMCA			1.000	μ mol·l ⁻¹ ·s ⁻¹	\overline{Z}
q			2.000	dimensionless	$\overline{\mathbf{Z}}$
K_PMCA			0.450	μ mol·l ⁻¹	$\overline{\mathbf{Z}}$
V_PLC			0.500	μ mol·l ⁻¹ ·s ⁻¹	$\overline{\mathbf{Z}}$
K_PLC			0.120	μ mol·l ⁻¹	$\overline{\mathbf{Z}}$
kdeg			0.500	s^{-1}	\overline{Z}
K_{-} deg			0.100	μ mol·l ⁻¹	\overline{Z}
A			0.500	$\mu \text{mol}^{-1} \cdot 1 \cdot \text{s}^{-1}$	$\overline{\mathbf{Z}}$
Kd			0.400	μ mol·l ⁻¹	\overline{Z}
K1			5.000	μ mol·l ⁻¹	$\overline{\mathbf{Z}}$
St			0.600	μ mol·l ⁻¹	$\overline{\mathbf{Z}}$
k_a			4.000	s^{-1}	$\overline{\mathbf{Z}}$
Vs4			0.250	$\mu mol \cdot l^{-1} \cdot s^{-1}$	$\overline{\mathbf{Z}}$
K2			0.140	μ mol·l ⁻¹	$ \overline{\mathbf{Z}} $
$\mathtt{kd_oligo}$			0.800	s^{-1}	
Vcp			$1.8 \cdot 10^{-4}$	$\mu \text{mol} \cdot l^{-1} \cdot s^{-1}$	$\overline{\mathbf{Z}}$
n_hill			3.000	dimensionless	$\overline{\mathbf{Z}}$
Kc			$2 \cdot 10^{-5}$	μ mol·l ⁻¹	$\overline{\mathbf{Z}}$
kdc			0.500	s^{-1}	\overline{Z}
kop			0.500	s^{-1}	$\overline{\mathbf{Z}}$
l_hill			1.000	dimensionless	$\overline{\mathbf{Z}}$
Ko			0.200	$\mu mol \cdot l^{-1}$	$\overline{\mathbf{Z}}$
kod			1.000	s^{-1}	\overline{Z}
kdo			0.600	s^{-1}	$\overline{\mathbf{Z}}$
r_hill			4.000	dimensionless	\overline{Z}
h			0.000	dimensionless	

Id	Name	SBO	Value	Unit	Constant
Orai1_t			0.001	$\mu mol \cdot l^{-1}$	

6 Rules

This is an overview of three rules.

6.1 Rule Orai1

Rule Orai1 is an assignment rule for species Orai1:

$$Orai1 = Orai1_t - (r_hill \cdot [Oc] + r_hill \cdot [O_o])$$
 (1)

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

6.2 Rule S2

Rule S2 is an assignment rule for species S2:

$$S2 = \frac{K1^2}{[Ca_ER]^2 + K1^2} \cdot (St - [S2a])$$
 (2)

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

6.3 Rule h

Rule h is a rate rule for parameter h:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{h} = \mathbf{A} \cdot (\mathbf{K}\mathbf{d} - ([\mathbf{C}\mathbf{a}_{-}\mathbf{C}\mathbf{y}\mathbf{t}] + \mathbf{K}\mathbf{d}) \cdot \mathbf{h}) \tag{3}$$

Derived unit $\,\mathrm{s}^{-1}$

7 Reactions

This model contains 15 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

$N\!$	Id	Name	Reaction Equation	SBO
1	ER_Channel		$Ca_ER \xrightarrow{IP3_Cyt} Ca_Cyt$	
2			•	
2	SERCA		$Ca_Cyt \longrightarrow Ca_ER$	
3	$PM_Channel$		$\emptyset \xrightarrow{Oo} Ca_Cyt$	
4	PMCA		$Ca_{-}Cyt \longrightarrow \emptyset$	
5	PLC		$\emptyset \xrightarrow{\text{Ca_Cyt}} \text{IP3_Cyt}$	
6	deg		$IP3_Cyt \xrightarrow{Ca_Cyt} \emptyset$	
7	act_apoSTIM1-		$\emptyset \xrightarrow{S2} S2a$	
	_syn			
8	act_apoSTIM1-		$S2a \longrightarrow \emptyset$	
	_deg			
9	apoSTIM1_oligo-		$\emptyset \xrightarrow{S2} S4$	
	_syn			
10	apoSTIM1_oligo-		$S4 \longrightarrow \emptyset$	
10	_deg			
			Orai1	
11	${\tt close_CRAC_prod}$		$\emptyset \xrightarrow{\operatorname{Orail}} \operatorname{Oc}$	
12	closed_CRAC-		$Oc \longrightarrow \emptyset$	
	$_{\tt channel_deg}$			
13	open_CRAC-		$Oc \xrightarrow{S2a} O_{-o}$	
	_channel_prod			
	_ondinor_prod			

N⁰	Id	Name	Reaction Equation	SBO
14	$open_to_closed$		$O_o \longrightarrow Oc$	
15	open_CRAC- _channel_deg		$O_{-}o \longrightarrow \emptyset$	

7.1 Reaction ER_Channel

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

Reaction equation

$$Ca_ER \xrightarrow{IP3_Cyt} Ca_Cyt$$
 (4)

Reactant

Table 6: Properties of each reactant.

Id	Name	SBO
Ca_ER		

Modifier

Table 7: Properties of each modifier.

Id	Name	SBO
IP3_Cyt		

Product

Table 8: Properties of each product.

Id	Name	SBO
Ca_Cyt		

Kinetic Law

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

$$v_{1} = vol\left(Cytoplasm\right) \cdot \left(L + \frac{P_IP3R \cdot [IP3_Cyt]^{3} \cdot [Ca_Cyt]^{3} \cdot h^{3}}{\left([IP3_Cyt] + Ki\right)^{3} \cdot \left([Ca_Cyt] + Ka\right)^{3}}\right) \cdot \left([Ca_ER] - [Ca_Cyt]\right) \tag{5}$$

7.2 Reaction SERCA

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

Reaction equation

$$Ca_Cyt \longrightarrow Ca_ER$$
 (6)

Reactant

Table 9: Properties of each reactant.

Id	Name	SBO
Ca_Cyt		

Product

Table 10: Properties of each product.

Id	Name	SBO
Ca_ER		

Kinetic Law

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

$$v_2 = \text{vol}\left(\text{Cytoplasm}\right) \cdot \frac{\text{V_SERCA} \cdot [\text{Ca_Cyt}]^p}{\text{K_SERCA}^p + [\text{Ca_Cyt}]^p}$$
(7)

7.3 Reaction PM_Channel

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

Reaction equation

$$\emptyset \xrightarrow{O_o} Ca_Cyt \tag{8}$$

Modifier

Table 11: Properties of each modifier.

Id	Name	SBO
0_0		

Product

Table 12: Properties of each product.

Id	Name	SBO
Ca_Cyt		

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

$$v_3 = \text{vol}\left(\text{Cytoplasm}\right) \cdot \left(\text{k_soc} \cdot [\text{O_o}] + \text{V_PMleak}\right) \cdot \left(\text{Ca_ec} - [\text{Ca_Cyt}]\right)$$
 (9)

7.4 Reaction PMCA

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

Reaction equation

$$Ca_Cyt \longrightarrow \emptyset \tag{10}$$

Reactant

Table 13: Properties of each reactant.

Id	Name	SBO
Ca_Cyt		

Kinetic Law

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

$$v_{4} = vol\left(Cytoplasm\right) \cdot \frac{V_PMCA \cdot [Ca_Cyt]^{q}}{K_PMCA^{q} + [Ca_Cyt]^{q}}$$
(11)

7.5 Reaction PLC

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

Reaction equation

$$\emptyset \xrightarrow{\text{Ca_Cyt}} \text{IP3_Cyt}$$
 (12)

Modifier

Table 14: Properties of each modifier.

Id	Name	SBO
Ca_Cyt		

Product

Table 15: Properties of each product.

Id	Name	SBO
IP3_Cyt		

Kinetic Law

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

$$v_5 = \text{vol}\left(\text{Cytoplasm}\right) \cdot \frac{\text{V_PLC} \cdot [\text{Ca_Cyt}]^2}{\text{K_PLC}^2 + [\text{Ca_Cyt}]^2}$$
(13)

7.6 Reaction deg

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

Reaction equation

$$IP3_Cyt \xrightarrow{Ca_Cyt} \emptyset$$
 (14)

Reactant

Table 16: Properties of each reactant.

Id	Name	SBO
IP3_Cyt		

Modifier

Table 17: Properties of each modifier.

Id	Name	SBO
Ca_Cyt		

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

$$v_6 = vol(Cytoplasm) \cdot \frac{kdeg \cdot [Ca_Cyt]^2}{K_deg^2 + [Ca_Cyt]^2} \cdot [IP3_Cyt]$$
 (15)

7.7 Reaction act_apoSTIM1_syn

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

Reaction equation

$$\emptyset \xrightarrow{S2} S2a \tag{16}$$

Modifier

Table 18: Properties of each modifier.

Id	Name	SBO
S2		

Product

Table 19: Properties of each product.

Id	Name	SBO
S2a		

Kinetic Law

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

$$v_7 = \text{vol}(\text{ER}) \cdot \mathbf{k}_{-}\mathbf{a} \cdot [\text{S2}] \tag{17}$$

7.8 Reaction act_apoSTIM1_deg

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

Reaction equation

$$S2a \longrightarrow \emptyset \tag{18}$$

Reactant

Table 20: Properties of each reactant.

Id	Name	SBO
S2a		

Kinetic Law

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

$$v_8 = \text{vol}(\text{ER}) \cdot \text{k.i.} [\text{S2a}]$$
 (19)

7.9 Reaction apoSTIM1_oligo_syn

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

Reaction equation

$$\emptyset \xrightarrow{S2} S4 \tag{20}$$

Modifier

Table 21: Properties of each modifier.

Id	Name	SBO
S2		

Product

Table 22: Properties of each product.

Id	Name	SBO
S4		

Kinetic Law

Derived unit $1.000000000000024 \cdot 10^{-6} \ mol \cdot s^{-1}$

$$v_9 = \text{vol}(\text{ER}) \cdot \frac{\text{Vs4} \cdot [\text{S2}]^2}{[\text{S2}]^2 + \text{K2}^2}$$
 (21)

7.10 Reaction apoSTIM1_oligo_deg

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

Reaction equation

$$S4 \longrightarrow \emptyset$$
 (22)

Reactant

Table 23: Properties of each reactant.

Id	Name	SBO
S4		

Kinetic Law

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

$$v_{10} = \text{vol}(\text{ER}) \cdot \text{kd_oligo} \cdot [\text{S4}]$$
 (23)

7.11 Reaction close_CRAC_prod

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

Reaction equation

$$\emptyset \xrightarrow{\text{Orail}} \text{Oc}$$
 (24)

Modifier

Table 24: Properties of each modifier.

Id	Name	SBO
Orai1		

Product

Table 25: Properties of each product.

Id	Name	SBO
Оc		

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

$$v_{11} = \text{vol}(PM) \cdot \frac{\text{Vcp} \cdot [\text{Orai1}]^{\text{n-hill}}}{\text{Kc}^{\text{n-hill}} + [\text{Orai1}]^{\text{n-hill}}}$$
(25)

7.12 Reaction closed_CRAC_channel_deg

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

Reaction equation

$$Oc \longrightarrow \emptyset$$
 (26)

Reactant

Table 26: Properties of each reactant.

Id	Name	SBO
0c		

Kinetic Law

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

$$v_{12} = \text{vol}(PM) \cdot \text{kdc} \cdot [Oc]$$
 (27)

7.13 Reaction open_CRAC_channel_prod

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

Reaction equation

$$Oc \xrightarrow{S2a} O_{-o}$$
 (28)

Reactant

Table 27: Properties of each reactant.

Id	Name	SBO
0c		

Modifier

Table 28: Properties of each modifier.

Id	Name	SBO
S2a		

Product

Table 29: Properties of each product.

Id	Name	SBO
0_0		

Kinetic Law

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

$$v_{13} = \text{vol}(PM) \cdot \frac{\text{kop} \cdot [S2a]^{l\text{-hill}} \cdot [Oc]}{\text{Ko}^{l\text{-hill}} + [S2a]^{l\text{-hill}}}$$
(29)

7.14 Reaction open_to_closed

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

Reaction equation

$$O_{-}o \longrightarrow Oc$$
 (30)

Reactant

Table 30: Properties of each reactant.

Id	Name	SBO
0_0		

Product

Table 31: Properties of each product.

Id	Name	SBO
Ос		

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

$$v_{14} = \text{vol}(PM) \cdot \text{kod} \cdot [O_o] \tag{31}$$

7.15 Reaction open_CRAC_channel_deg

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

Reaction equation

$$O_{-}o \longrightarrow \emptyset$$
 (32)

Reactant

Table 32: Properties of each reactant.

Id	Name	SBO
0_0		

Kinetic Law

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

$$v_{15} = \text{vol}(PM) \cdot \text{kdo} \cdot [O_o] \tag{33}$$

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.

8.1 Species Ca_Cyt

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

This species takes part in six reactions (as a reactant in SERCA, PMCA and as a product in ER-_Channel, PM_Channel and as a modifier in PLC, deg).

$$\frac{d}{dt}Ca_{-}Cyt = v_1 + v_3 - v_2 - v_4 \tag{34}$$

8.2 Species IP3_Cyt

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

This species takes part in three reactions (as a reactant in deg and as a product in PLC and as a modifier in ER_Channel).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{IP3}_{-}\mathrm{Cyt} = v_5 - v_6 \tag{35}$$

8.3 Species Ca_ER

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

This species takes part in two reactions (as a reactant in ER_Channel and as a product in SERCA).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Ca}_{-}\mathrm{ER} = v_2 - v_1 \tag{36}$$

8.4 Species S2

Initial concentration $0.54 \mu mol \cdot l^{-1}$

Involved in rule S2

This species takes part in two reactions (as a modifier in act_apoSTIM1_syn, apoSTIM1_oligo_syn) and is also involved in one rule which determines this species' quantity.

8.5 Species S2a

Initial concentration $0.06 \ \mu mol \cdot l^{-1}$

This species takes part in three reactions (as a reactant in act_apoSTIM1_deg and as a product in act_apoSTIM1_syn and as a modifier in open_CRAC_channel_prod).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{S}2\mathrm{a} = v_7 - v_8 \tag{37}$$

8.6 Species S4

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

This species takes part in two reactions (as a reactant in apoSTIM1_oligo_deg and as a product in apoSTIM1_oligo_syn).

$$\frac{d}{dt}S4 = v_9 - v_{10} \tag{38}$$

8.7 Species Oc

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

This species takes part in four reactions (as a reactant in closed_CRAC_channel_deg, open_CRAC_channel_prod and as a product in close_CRAC_prod, open_to_closed).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Oc} = v_{11} + v_{14} - v_{12} - v_{13} \tag{39}$$

8.8 Species O_o

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

This species takes part in four reactions (as a reactant in open_to_closed, open_CRAC_channel_deg and as a product in open_CRAC_channel_prod and as a modifier in PM_Channel).

$$\frac{\mathrm{d}}{\mathrm{d}t}O_{-}o = v_{13} - v_{14} - v_{15} \tag{40}$$

8.9 Species Orai1

Initial concentration $0.0010~\mu mol \cdot l^{-1}$

Involved in rule Orai1

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

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