SBML Model Report

Model name: "Chay1997_CalciumConcentration"

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: Ishan Ajmera[1] and Catherine Lloyd[2] at September 29th 2011 at 10:17 p. m. and last time modified at April eighth 2016 at 5:08 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	1
species types	0	species	6
events	0	constraints	0
reactions	0	function definitions	0
global parameters	49	unit definitions	0
rules	21	initial assignments	0

Model Notes

This a model from the article:
Effects of extracellular calcium on electrical bursting and intracellular and luminal calcium oscillations in insulin secreting pancreatic beta-cells.
Chay TR Biophys J.1997 Sep;73(3):1673-88. 9284334,

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Abstract:
The extracellular calcium concentration has interesting effects on bursting of pancreatic beta-cells. The mechanism underlying the extracellular Ca2+ effect is not well understood. By incorporating a low-threshold transient inward current to the store-operated bursting model of Chay, this paper elucidates the role of the extracellular Ca2+ concentration in influencing electrical activity, intracellular Ca2+ concentration, and the luminal Ca2+ concentration in the intracellular Ca2+ store. The possibility that this inward current is a carbachol-sensitive and TTX-insensitive Na+ current discovered by others is discussed. In addition, this paper explains how these three variables respond when various pharmacological agents are applied to the store-operated model.

This model was taken from the CellML repository and automatically converted to SBML.
The original model was: **Chay TR (1997) - version05**
The original CellML model was created by:
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To cite BioModels Database, please use: Li C, Donizelli M, Rodriguez N, Dharuri H, Endler L, Chelliah V, Li L, He E, Henry A, Stefan MI, Snoep JL, Hucka M, Le Novre N, Laibe C (2010) BioModels Database: An enhanced, curated and annotated resource for published quantitative kinetic models. BMC Syst Biol., 4:92.

2 Unit Definitions

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

2.1 Unit substance

Notes Mole is the predefined SBML unit for substance.

Definition mol

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 Compartment

This model contains one compartment.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
`Compartment`	Compartment		3	1	litre	☑	

3.1 Compartment `Compartment`

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

Name Compartment

4 Species

This model contains six 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
`V_membrane`	V_membrane	`Compartment`	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	$\boxminus$	$\boxminus$
`h`	h	`Compartment`	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	$\boxminus$	$\boxminus$
`d`	d	`Compartment`	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	$\boxminus$	$\boxminus$
`n`	n	`Compartment`	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	$\boxminus$	$\boxminus$
`Ca_i_cytosolic_calcium`	Ca_i_cytosolic_calcium	`Compartment`	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	$\boxminus$	$\boxminus$
`Ca_lum`	Ca_lum	`Compartment`	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	$\boxminus$	$\boxminus$

5 Parameters

This model contains 49 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
R	R	0000567	8314.000		☑
T	T	0000002	310.000		☑
F	F	0000568	96485.000		☑
Cm	Cm	0000247	1.000		☑
i_fast	i_fast		−96.640		☐
g_fast	g_fast	0000009	600.000		☑
V_fast	V_fast	0000009	80.000		☑
m_infinity	m_infinity	0000009	0.185		☐
Vm	Vm	0000009	−25.000		☑
Sm	Sm	0000009	9.000		☑
lamda_h	lamda_h		12.500		☑
tau_h	tau_h	0000009	0.032		☐
h_infinity	h_infinity	0000009	0.201		☐
Vh	Vh	0000009	−48.000		☑
Sh	Sh	0000009	−7.000		☑
i_Ca	i_Ca	0000009	−24.125		☐
K_Ca	K_Ca	0000009	1.000		☑
P_Ca	P_Ca	0000009	2.000		☑
Ca_o	Ca_o	0000009	2500.000		☑
lamda_d	lamda_d	0000009	2.500		☑
tau_d	tau_d		0.023		☐
d_infinity	d_infinity		0.003		☐
Vd	Vd	0000009	−10.000		☑
Sd	Sd	0000009	5.000		☑
f_infinity	f_infinity		0.500		☐
Ca_i-_calcium-_current_f-_gate	Ca_i		1.000		☑
i_NS	i_NS	0000009	−6.241		☐
g_NS	g_NS	0000009	5.000		☑
K_NS	K_NS	0000009	50.000		☑
VNS	VNS	0000009	−20.000		☑
i_K_dr	i_K_dr		25.015		☐
V_K	V_K	0000009	−75.000		☑
g_K_dr	g_K_dr	0000009	600.000		☑
lamda_n	lamda_n	0000009	12.500		☑

Id	Name	SBO	Value	Unit	Constant
Vn	Vn	0000009	-18.000		☑
Sn	Sn	0000009	14.000		☑
n_infinity	n_infinity		0.190		☐
tau_n	tau_n		0.031		☐
i_K_Ca	i_K_Ca		46.208		☐
g_K_Ca	g_K_Ca		5.000		☑
i_K_ATP	i_K_ATP		73.317		☐
g_K_ATP	g_K_ATP		2.000		☑
i_NaL	i_NaL		-35.502		☐
g_NaL	g_NaL	0000009	0.300		☑
V_Na	V_Na	0000009	80.000		☑
k_rel	k_rel	0000009	0.200		☑
k_Ca	k_Ca	0000009	7.000		☑
k_pump	k_pump	0000009	30.000		☑
omega	omega	0000009	0.200		☑

6 Rules

This is an overview of 21 rules.

6.1 Rule m_infinity

Rule m_infinity is an assignment rule for parameter m_infinity:

$$\text{m\_infinity} = \frac{1}{1 + \exp\left(\frac{\text{Vm} - [\text{V\_membrane}]}{\text{Sm}}\right)} \tag{1}$$

6.2 Rule i_fast

Rule i_fast is an assignment rule for parameter i_fast:

$$\text{i\_fast} = \text{g\_fast} \cdot \text{m\_infinity}^{3} \cdot [\text{h}] \cdot ([\text{V\_membrane}] - \text{V\_fast}) \tag{2}$$

6.3 Rule tau_h

Rule tau_h is an assignment rule for parameter tau_h:

$$\text{tau\_h} = \frac{1}{\text{lamda\_h} \cdot \left(\exp\left(\frac{\text{Vh} - [\text{V\_membrane}]}{2 \cdot \text{Sh}}\right) + \exp\left(\frac{[\text{V\_membrane}] - \text{Vh}}{2 \cdot \text{Sh}}\right)\right)} \tag{3}$$

6.4 Rule h_infinity

Rule h_infinity is an assignment rule for parameter h_infinity:

$$\text{h\_infinity} = \frac{1}{1 + \exp\left(\frac{\text{Vh} - [\text{V\_membrane}]}{\text{Sh}}\right)} \tag{4}$$

6.5 Rule tau_d

Rule tau_d is an assignment rule for parameter tau_d:

$$\text{tau\_d} = \frac{1}{\text{lamda\_d} \cdot \left(\exp\left(\frac{\text{Vd} - [\text{V\_membrane}]}{2 \cdot \text{Sd}}\right) + \exp\left(\frac{[\text{V\_membrane}] - \text{Vd}}{2 \cdot \text{Sd}}\right)\right)} \tag{5}$$

6.6 Rule f_infinity

Rule f_infinity is an assignment rule for parameter f_infinity:

$$\text{f\_infinity} = \frac{\text{K\_Ca}}{\text{K\_Ca} + \text{Ca\_i\_calcium\_current\_f\_gate}} \tag{6}$$

6.7 Rule i_Ca

Rule i_Ca is an assignment rule for parameter i_Ca:

$$\text{i\_Ca} = \frac{\frac{\text{P\_Ca} \cdot [\text{d}] \cdot \text{f\_infinity} \cdot 2 \cdot \text{F} \cdot [\text{V\_membrane}]}{\text{R} \cdot \text{T}} \cdot \left(\text{Ca\_o} - [\text{Ca\_i\_cytosolic\_calcium}] \cdot \exp\left(\frac{2 \cdot \text{F} \cdot [\text{V\_membrane}]}{\text{R} \cdot \text{T}}\right)\right)}{1 - \exp\left(\frac{2 \cdot \text{F} \cdot [\text{V\_membrane}]}{\text{R} \cdot \text{T}}\right)} \tag{7}$$

6.8 Rule d_infinity

Rule d_infinity is an assignment rule for parameter d_infinity:

$$\text{d\_infinity} = \frac{1}{1 + \exp\left(\frac{\text{Vd} - [\text{V\_membrane}]}{\text{Sd}}\right)} \tag{8}$$

6.9 Rule i_NS

Rule i_NS is an assignment rule for parameter i_NS:

$$\text{i\_NS} = \frac{\text{g\_NS} \cdot \text{K\_NS}^2}{\text{K\_NS}^2 + [\text{Ca\_lum}]^2} \cdot \left(\frac{[\text{V\_membrane}] - \text{VNS}}{1 - \exp\left(0.1 \cdot (\text{VNS} - [\text{V\_membrane}])\right)} - 10\right) \tag{9}$$

6.10 Rule i_K_dr

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

$$\text{i\_K\_dr} = \text{g\_K\_dr} \cdot [\text{n}]^4 \cdot ([\text{V\_membrane}] - \text{V\_K}) \tag{10}$$

6.11 Rule n_infinity

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

$$\text{n\_infinity} = \frac{1}{1 + \exp\left(\frac{\text{Vn} - [\text{V\_membrane}]}{\text{Sn}}\right)} \tag{11}$$

6.12 Rule tau_n

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

$$\text{tau\_n} = \frac{1}{\text{lamda\_n} \cdot \left(\exp\left(\frac{\text{Vn} - [\text{V\_membrane}]}{2 \cdot \text{Sn}}\right) + \exp\left(\frac{[\text{V\_membrane}] - \text{Vn}}{2 \cdot \text{Sn}}\right)\right)} \tag{12}$$

6.13 Rule i_K_ATP

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

$$\text{i\_K\_ATP} = \text{g\_K\_ATP} \cdot ([\text{V\_membrane}] - \text{V\_K}) \tag{13}$$

6.14 Rule i_K_Ca

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

$$\text{i\_K\_Ca} = \frac{\text{g\_K\_Ca} \cdot [\text{Ca\_i\_cytosolic\_calcium}]^3}{\text{K\_Ca}^3 + [\text{Ca\_i\_cytosolic\_calcium}]^3} \cdot ([\text{V\_membrane}] - \text{V\_K}) \tag{14}$$

6.15 Rule i_NaL

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

$$\text{i\_NaL} = \text{g\_NaL} \cdot ([\text{V\_membrane}] - \text{V\_Na}) \tag{15}$$

6.16 Rule V_membrane

Rule `V_membrane` is a rate rule for species `V_membrane`:

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{V\_membrane} = \frac{(\text{i\_K\_dr} + \text{i\_K\_Ca} + \text{i\_K\_ATP} + \text{i\_fast} + \text{i\_Ca} + \text{i\_NS} + \text{i\_NaL})}{\text{Cm}} \tag{16}$$

6.17 Rule h

Rule h is a rate rule for species h:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{h} = \frac{\mathrm{h\_infinity} - [\mathrm{h}]}{\mathrm{tau\_h}} \tag{17}$$

6.18 Rule d

Rule d is a rate rule for species d:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{d} = \frac{\mathrm{d\_infinity} - [\mathrm{d}]}{\mathrm{tau\_d}} \tag{18}$$

6.19 Rule n

Rule n is a rate rule for species n:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{n} = \frac{\mathrm{n\_infinity} - [\mathrm{n}]}{\mathrm{tau\_n}} \tag{19}$$

6.20 Rule Ca_i_cytosolic_calcium

Rule Ca_i_cytosolic_calcium is a rate rule for species Ca_i_cytosolic_calcium:

$$\begin{split}\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Ca\_i\_cytosolic\_calcium} = \mathrm{k\_rel} \cdot ([\mathrm{Ca\_lum}] - [\mathrm{Ca\_i\_cytosolic\_calcium}]) - (\mathrm{omega} \cdot \mathrm{i\_Ca} + \mathrm{k\_Ca} \\ \cdot [\mathrm{Ca\_i\_cytosolic\_calcium}] + \mathrm{k\_pump} \cdot [\mathrm{Ca\_i\_cytosolic\_calcium}])\end{split} \tag{20}$$

6.21 Rule Ca_lum

Rule Ca_lum is a rate rule for species Ca_lum:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Ca\_lum} = \mathrm{k\_rel} \cdot ([\mathrm{Ca\_lum}] - [\mathrm{Ca\_i\_cytosolic\_calcium}]) + \mathrm{k\_pump} \cdot [\mathrm{Ca\_i\_cytosolic\_calcium}] \tag{21}$$

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 V_membrane

Name V_membrane

SBO:0000259 voltage

Initial amount -38.34146 mol

Involved in rule V_membrane

One rule which determines this species' quantity.

7.2 Species h

Name h

Initial amount 0.214723 mol

Involved in rule h

One rule which determines this species' quantity.

7.3 Species d

Name d

Initial amount 0.0031711238 mol

Involved in rule d

One rule which determines this species' quantity.

7.4 Species n

Name n

Initial amount 0.1836403 mol

Involved in rule n

One rule which determines this species' quantity.

7.5 Species Ca_i_cytosolic_calcium

Name Ca_i_cytosolic_calcium

Initial amount 0.6959466 mol

Involved in rule Ca_i_cytosolic_calcium

One rule which determines this species' quantity.

7.6 Species Ca_lum

Name Ca_lum

Initial amount 102.686 mol

Involved in rule Ca_lum

One rule which determines this species' quantity.

A Glossary of Systems Biology Ontology Terms

SBO:0000002 quantitative systems description parameter: A numerical value that defines certain characteristics of systems or system functions. It may be part of a calculation, but its value is not determined by the form of the equation itself, and may be arbitrarily assigned

SBO:0000009 kinetic constant: Numerical parameter that quantifies the velocity of a chemical reaction

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

SBO:0000259 voltage: Difference of electrical potential between two points of an electrical network, expressed in volts

SBO:0000567 universal gas constant: A physical constant featured in many fundamental equations in the physical sciences. It is equivalent to the Boltzmann constant, but expressed in units of energy per temperature increment per mole (rather than energy per temperature increment per particle). It has the value 8.314 J.K-1.mol-1 and is denoted by the symbol R

SBO:0000568 Faraday constant: Named after Michael Faraday, it is the magnitude of electric charge per mole of electrons. It has the value 96,485.3365 C/mol (Coulombs per Mole), and the symbol F

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