SBML Model Report

Model name: "Fridlyand2003_Calcium_flux"

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 June 20th 2006 at 1:12 p. m. and last time modified at May 24th 2014 at 4:27 p. 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	6
events	0	constraints	0
reactions	18	function definitions	0
global parameters	97	unit definitions	17
rules	37	initial assignments	0

Model Notes

The model reproduces block A of Fig 5 and also Fig 3 (without the inclusion of Tg action). The model was successfully tested on MathSBML

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commercially or not, in a restricted way or not.

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 20 unit definitions of which three are predefined by SBML and not mentioned in the model.

2.1 Unit `substance`

Name Micromole

Definition µmol

2.2 Unit `time`

Name milliseconds

Definition ms

2.3 Unit `millivolt`

Name Voltage

Definition mV

2.4 Unit `femtoamperes`

Name Current

Definition fA

2.5 Unit `micromole_per_litre`

Name Concentration

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

2.6 Unit `picosiemens`

Name Conductance

Definition pS

2.7 Unit femtofarads

Name Capacitance

Definition fF

2.8 Unit per_millisecond

Name Time inverse

Definition ms^{-1}

2.9 Unit picosiemens_per_millivolt

Name Conductance coefficient

Definition $\mathrm{pS} \cdot \mathrm{mV}^{-1}$

2.10 Unit micromole_per_millisecond

Name amount per time

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

2.11 Unit microM_per_millisecond

Name concentration per time

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

2.12 Unit litres_per_millisecond

Name volume per time

Definition $\mathrm{l} \cdot \mathrm{ms}^{-1}$

2.13 Unit per_microM_per_millisecond

Name per concentration per time

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

2.14 Unit per_microMcube_per_millisecond

Name per concentration cubed per time

Definition $\mu\mathrm{mol}^{-3} \cdot \mathrm{ms}^{-1} \cdot \mathrm{l}^{3}$

2.15 Unit per_microMsquare_per_millisecond

Name per Concentration square per time

Definition $\mu mol^{-2} \cdot ms^{-1} \cdot l^{2}$

2.16 Unit per_microM

Name per concentration

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

2.17 Unit fA_msec_per_micromole

Name Faraday constant

Definition $fA \cdot ms \cdot \mu mol^{-1}$

2.18 Unit volume

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

Definition l

2.19 Unit area

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

Definition m^2

2.20 Unit length

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

Definition m

3 Compartments

This model contains two compartments.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
Cytoplasm	cytoplasm		3	$7.64 \cdot 10^{-13}$	l	☑	
ER	endoplasmic reticulum		3	$2.8 \cdot 10^{-13}$	l	☑	Cytoplasm

3.1 Compartment `Cytoplasm`

This is a three dimensional compartment with a constant size of $7.64 \cdot 10^{-13}$ litre.

Name cytoplasm

3.2 Compartment `ER`

This is a three dimensional compartment with a constant size of $2.8 \cdot 10^{-13}$ litre, which is surrounded by `Cytoplasm` (cytoplasm).

Name endoplasmic reticulum

4 Species

This model contains six 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
Ca_cyt	Cytosolic Calcium	Cytoplasm	$\mu mol \cdot l^{-1}$	⊟	⊟
Ca_er	ER Calcium	ER	$\mu mol \cdot l^{-1}$	⊟	⊟
IP3_cyt	Cytosolic IP3	Cytoplasm	$\mu mol \cdot l^{-1}$	⊟	⊟
Na_cyt	Cytosolic Sodium	Cytoplasm	$\mu mol \cdot l^{-1}$	⊟	⊟
ATP_cyt	Cytosolic ATP	Cytoplasm	$\mu mol \cdot l^{-1}$	⊟	⊟
ADP_cyt	Cytosolic ADP	Cytoplasm	$\mu mol \cdot l^{-1}$	⊟	⊟

5 Parameters

This model contains 97 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
n			0.001		☐
V			−60.900	mV	☐
Vca			0.000	mV	☐
TV			26.730	mV	☑
Ca_ec			2600.000	$\mu mol \cdot l^{-1}$	☑
Vk			0.000	mV	☐
K_ec			8000.000	$\mu mol \cdot l^{-1}$	☑
K_cyt			132400.000	$\mu mol \cdot l^{-1}$	☑
Vna			0.000	mV	☐
Na_ec			140000.000	$\mu mol \cdot l^{-1}$	☑
Vnaca			0.000	mV	☐
pvca			0.000		☐
Vcah			−19.000	mV	☑
Kcah			9.500	mV	☑
f_CRAN			0.000		☐
gm_CRAN			0.700	$pS \cdot mV^{-1}$	☑
Kcar			200.000	$\mu mol \cdot l^{-1}$	☑
p_CRAN			0.000	mV	☐
V_CRAN			0.000	mV	☑
pna			0.000	dimensionless	☐
f_5			0.000		☐
f5_ast			0.002	$\mu mol^{-1} \cdot ms^{-1} \cdot 1$	☑
b_5			0.000		☐
b5_ast			0.030	ms^{-1}	☑
F1			0.000		☐
f_1			$2.5 \cdot 10^{-10}$	$\mu mol^{-3} \cdot ms^{-1} \cdot l^{3}$	☑
F4			0.000		☐
f_4			$1.5 \cdot 10^{-8}$	$\mu mol^{-2} \cdot ms^{-1} \cdot l^{2}$	☑
F5			0.000		☐
B2			0.000		☐
b_2			10^{-4}	$\mu mol^{-1} \cdot ms^{-1} \cdot 1$	☑
B3			0.000		☐
b_3			$1.72 \cdot 10^{-17}$	$\mu mol^{-3} \cdot ms^{-1} \cdot l^{3}$	☑
B4			0.000		☐
b_4			$2 \cdot 10^{-4}$	$\mu mol^{-1} \cdot ms^{-1} \cdot 1$	☑
P			4950.000	$\mu mol \cdot l^{-1}$	☑

Id	Name	SBO	Value	Unit	Constant
B6			0.000		☐
b_6			$6 \cdot 10^{-7}$	$\mu mol^{-1} \cdot ms^{-1} \cdot l$	☑
Ksup			150400.000	$\mu mol \cdot l^{-1}$	☑
D			0.000		☐
f_2			10.000	ms^{-1}	☑
f_3			0.172	ms^{-1}	☑
f_6			11.500	ms^{-1}	☑
b_1			100.000	ms^{-1}	☑
f_Ca			0.000	dimensionless	☐
Kkca			0.100	$\mu mol \cdot l^{-1}$	☑
Okatp			0.000	dimensionless	☐
Kdd			17.000	$\mu mol \cdot l^{-1}$	☑
Ktd			26.000	$\mu mol \cdot l^{-1}$	☑
Ktt			1.000	$\mu mol \cdot l^{-1}$	☑
n_infinity			0.000	dimensionless	☐
Vn			−14.000	mV	☑
Sn			7.000	mV	☑
tau_n			0.000	ms	☐
c			20.000	ms	☑
Vtau			−75.000	mV	☑
a			65.000	mV	☑
b			20.000	mV	☑
I_Vca			0.000	fA	☐
gmvca			770.000	pS	☑
I_CaPump			0.000	fA	☐
Pmcap			2000.000	fA	☑
Kcap			0.100	$\mu mol \cdot l^{-1}$	☑
I_NaCa			0.000	fA	☐
gnaca			271.000	pS	☑
Knaca			0.750	$\mu mol \cdot l^{-1}$	☑
I_CRAN			0.000	fA	☐
I_Na			0.000	fA	☐
gmna			1200.000	pS	☑
I_NaK			0.000	fA	☐
Pnak			600.000	fA	☑
I_KDr			0.000	fA	☐
gmKDr			3000.000	pS	☑
I_KCa			0.000	fA	☐
gmkca			130.000	pS	☑
I_KATP			0.000	fA	☐
gmkatp			24000.000	pS	☑
Jerp			0.000	$\mu mol \cdot ms^{-1} \cdot l^{-1}$	☐

Id	Name	SBO	Value	Unit	Constant
Pcaer			0.105	$\mu mol \cdot ms^{-1} \cdot l^{-1}$	⊟
Kcarp			0.500	$\mu mol \cdot l^{-1}$	☑
O_infinity			0.000	dimensionless	⊟
Krca			0.077	$\mu mol \cdot l^{-1}$	☑
Kip3			3.200	$\mu mol \cdot l^{-1}$	☑
Jout			0.000	$\mu mol \cdot ms^{-1}$	⊟
Pleak			10^{-16}	$l \cdot ms^{-1}$	☑
Pip3			$1.2 \cdot 10^{-15}$	$l \cdot ms^{-1}$	☑
Cm			6158.000	fF	☑
fi			0.010	dimensionless	☑
F	Faraday's constant		$9.6485 \cdot 10^{16}$	$fA \cdot ms \cdot \mu mol^{-1}$	☑
ksg			10^{-4}	ms^{-1}	☑
fer			0.030	dimensionless	☑
kip	IP3 production rate constant		$3 \cdot 10^{-4}$	$\mu mol \cdot ms^{-1} \cdot l^{-1}$	☑
Kipca	half activation cytosolic Ca		0.400	$\mu mol \cdot l^{-1}$	☑
kdip	IP3 degradation rate constant		$4 \cdot 10^{-5}$	ms^{-1}	☑
kadp	ATP production rate constant		$3.7 \cdot 10^{-4}$	ms^{-1}	☑
katpca	Ca dependent ATP consumption		$5 \cdot 10^{-5}$	$\mu mol^{-1} \cdot ms^{-1} \cdot l$	☑
katp	Rate constant of ATP consumption		$5 \cdot 10^{-5}$	ms^{-1}	☑

6 Rules

This is an overview of 37 rules.

6.1 Rule ADP_cyt

Rule ADP_cyt is an assignment rule for species ADP_cyt:

$$\text{ADP\_cyt} = 4000 - [\text{ATP\_cyt}] \tag{1}$$

6.2 Rule Vca

Rule Vca is an assignment rule for parameter Vca:

$$\text{Vca} = \frac{\text{TV}}{2} \cdot \left(\frac{\text{Ca\_ec}}{[\text{Ca\_cyt}]} \right) \tag{2}$$

6.3 Rule Vk

Rule Vk is an assignment rule for parameter Vk:

$$\mathrm{Vk} = \mathrm{TV} \cdot \left(\frac{\mathrm{K\_ec}}{\mathrm{K\_cyt}} \right) \tag{3}$$

Derived unit mV

6.4 Rule Vna

Rule Vna is an assignment rule for parameter Vna:

$$\mathrm{Vna} = \mathrm{TV} \cdot \left(\frac{\mathrm{Na\_ec}}{[\mathrm{Na\_cyt}]} \right) \tag{4}$$

Derived unit mV

6.5 Rule Vnaca

Rule Vnaca is an assignment rule for parameter Vnaca:

$$\mathrm{Vnaca} = \mathrm{TV} \cdot \left(3 \cdot \left(\frac{\mathrm{Na\_ec}}{[\mathrm{Na\_cyt}]} \right) - \left(\frac{\mathrm{Ca\_ec}}{[\mathrm{Ca\_cyt}]} \right) \right) \tag{5}$$

6.6 Rule pvca

Rule pvca is an assignment rule for parameter pvca:

$$\mathrm{pvca} = \frac{1}{1 + \exp\left(\frac{\mathrm{Vcah} - \mathrm{V}}{\mathrm{Kcah}} \right)} \tag{6}$$

6.7 Rule f_CRAN

Rule f_CRAN is an assignment rule for parameter f_CRAN:

$$\mathrm{f\_CRAN} = \frac{\mathrm{gm\_CRAN}}{1 + \exp\left(\frac{[\mathrm{Ca\_er}] - \mathrm{Kcar}}{3} \right)} \tag{7}$$

6.8 Rule p_CRAN

Rule p_CRAN is an assignment rule for parameter p_CRAN:

$$\mathrm{p\_CRAN} = \mathrm{V} - \mathrm{V\_CRAN} \tag{8}$$

Derived unit mV

6.9 Rule pna

Rule pna is an assignment rule for parameter pna:

$$\text{pna} = \frac{1}{1 + \exp\left(\frac{104+\text{V}}{8}\right)} \tag{9}$$

6.10 Rule f_5

Rule f_5 is an assignment rule for parameter f_5:

$$\text{f\_5} = \text{f5\_ast} \cdot \exp\left(\frac{\text{V}}{2 \cdot \text{TV}}\right) \tag{10}$$

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

6.11 Rule b_5

Rule b_5 is an assignment rule for parameter b_5:

$$\text{b\_5} = \text{b5\_ast} \cdot \exp\left(\frac{\text{V}}{2 \cdot \text{TV}}\right) \tag{11}$$

Derived unit ms^{-1}

6.12 Rule F1

Rule F1 is an assignment rule for parameter F1:

$$\text{F1} = \text{f\_1} \cdot [\text{Na\_cyt}]^3 \tag{12}$$

Derived unit ms^{-1}

6.13 Rule F4

Rule F4 is an assignment rule for parameter F4:

$$\text{F4} = \text{f\_4} \cdot \text{K\_ec}^2 \tag{13}$$

Derived unit ms^{-1}

6.14 Rule F5

Rule F5 is an assignment rule for parameter F5:

$$\text{F5} = \text{f\_5} \cdot [\text{ATP\_cyt}] \tag{14}$$

6.15 Rule B2

Rule B2 is an assignment rule for parameter B2:

$$\mathrm{B2} = \mathrm{b\_2} \cdot [\mathrm{ADP\_cyt}] \tag{15}$$

Derived unit ms^{-1}

6.16 Rule B3

Rule B3 is an assignment rule for parameter B3:

$$\mathrm{B3} = \mathrm{b\_3} \cdot \mathrm{Na\_ec}^3 \tag{16}$$

Derived unit ms^{-1}

6.17 Rule B4

Rule B4 is an assignment rule for parameter B4:

$$\mathrm{B4} = \mathrm{b\_4} \cdot \mathrm{P} \tag{17}$$

Derived unit ms^{-1}

6.18 Rule B6

Rule B6 is an assignment rule for parameter B6:

$$\mathrm{B6} = \mathrm{b\_6} \cdot \mathrm{Ksup}^2 \tag{18}$$

Derived unit $10^{-6}\,\mathrm{mol} \cdot \mathrm{ms}^{-1} \cdot \mathrm{l}^{-1}$

6.19 Rule D

Rule D is an assignment rule for parameter D:

$$\begin{aligned}\mathrm{D} = {} & \mathrm{f\_2} \cdot \mathrm{f\_3} \cdot \mathrm{F4} \cdot \mathrm{F5} \cdot \mathrm{f\_6} + \mathrm{b\_1} \cdot \mathrm{f\_3} \cdot \mathrm{F4} \cdot \mathrm{F5} \cdot \mathrm{f\_6} + \mathrm{b\_1} \cdot \mathrm{B2} \cdot \mathrm{F4} \cdot \mathrm{F5} \cdot \mathrm{f\_6} \\ & + \mathrm{b\_1} \cdot \mathrm{B2} \cdot \mathrm{B3} \cdot \mathrm{F5} \cdot \mathrm{f\_6} + \mathrm{b\_1} \cdot \mathrm{B2} \cdot \mathrm{B3} \cdot \mathrm{B4} \cdot \mathrm{f\_6} + \mathrm{b\_1} \cdot \mathrm{B2} \cdot \mathrm{B3} \cdot \mathrm{B4} \cdot \mathrm{b\_5}\end{aligned} \tag{19}$$

6.20 Rule f_Ca

Rule f_Ca is an assignment rule for parameter f_Ca:

$$\mathrm{f\_Ca} = \frac{[\mathrm{Ca\_cyt}]^4}{[\mathrm{Ca\_cyt}]^4 + \mathrm{Kkca}^4} \tag{20}$$

Derived unit dimensionless

6.21 Rule Okatp

Rule Okatp is an assignment rule for parameter Okatp:

$$\text{Okatp} = \frac{0.08 \cdot \left(1 + 0.33 \cdot \frac{[\text{ADP\_cyt}]}{\text{Kdd}}\right) + 0.89 \cdot \left(0.165 \cdot \frac{[\text{ADP\_cyt}]}{\text{Kdd}}\right)^2}{\left(1 + 0.165 \cdot \frac{[\text{ADP\_cyt}]}{\text{Kdd}}\right)^2 \cdot \left(1 + 0.135 \cdot \frac{[\text{ADP\_cyt}]}{\text{Ktd}} + 0.05 \cdot \frac{[\text{ATP\_cyt}]}{\text{Ktt}}\right)} \tag{21}$$

6.22 Rule n_infinity

Rule n_infinity is an assignment rule for parameter n_infinity:

$$\text{n\_infinity} = \frac{1}{1 + \exp\left(\frac{\text{Vn} - \text{V}}{\text{Sn}}\right)} \tag{22}$$

6.23 Rule tau_n

Rule tau_n is an assignment rule for parameter tau_n:

$$\text{tau\_n} = \frac{\text{c}}{\exp\left(\frac{\text{V} - \text{Vtau}}{\text{a}}\right) + \exp\left(\frac{\text{Vtau} - \text{V}}{\text{b}}\right)} \tag{23}$$

Derived unit ms

6.24 Rule I_Vca

Rule I_Vca is an assignment rule for parameter I_Vca:

$$\text{I\_Vca} = \text{gmvca} \cdot \text{pvca} \cdot (\text{V} - \text{Vca}) \tag{24}$$

6.25 Rule I_CaPump

Rule I_CaPump is an assignment rule for parameter I_CaPump:

$$\text{I\_CaPump} = \frac{\text{Pmcap} \cdot [\text{Ca\_cyt}]^2}{\text{Kcap}^2 + [\text{Ca\_cyt}]^2} \tag{25}$$

Derived unit fA

6.26 Rule I_NaCa

Rule I_NaCa is an assignment rule for parameter I_NaCa:

$$\text{I\_NaCa} = \frac{\text{gnaca} \cdot [\text{Ca\_cyt}]^5 \cdot (\text{V} - \text{Vnaca})}{[\text{Ca\_cyt}]^5 + \text{Knaca}^5} \tag{26}$$

Derived unit pS · mV

6.27 Rule I_CRAN

Rule I_CRAN is an assignment rule for parameter I_CRAN:

$$\text{I\_CRAN} = \text{f\_CRAN} \cdot \text{p\_CRAN} \cdot (\text{V} - \text{Vna}) \tag{27}$$

6.28 Rule I_Na

Rule I_Na is an assignment rule for parameter I_Na:

$$\text{I\_Na} = \text{gmna} \cdot \text{pna} \cdot (\text{V} - \text{Vna}) \tag{28}$$

Derived unit $\text{pS} \cdot \text{mV}$

6.29 Rule I_NaK

Rule I_NaK is an assignment rule for parameter I_NaK:

$$\text{I\_NaK} = \frac{\text{Pnak} \cdot (\text{F1} \cdot \text{f\_2} \cdot \text{f\_3} \cdot \text{F4} \cdot \text{F5} \cdot \text{f\_6} - \text{b\_1} \cdot \text{B2} \cdot \text{B3} \cdot \text{B4} \cdot \text{b\_5} \cdot \text{B6})}{\text{D}} \tag{29}$$

6.30 Rule I_KDr

Rule I_KDr is an assignment rule for parameter I_KDr:

$$\text{I\_KDr} = \text{gmKDr} \cdot \text{n} \cdot (\text{V} - \text{Vk}) \tag{30}$$

6.31 Rule I_KCa

Rule I_KCa is an assignment rule for parameter I_KCa:

$$\text{I\_KCa} = \text{gmkca} \cdot \text{f\_Ca} \cdot (\text{V} - \text{Vk}) \tag{31}$$

Derived unit $\text{pS} \cdot \text{mV}$

6.32 Rule I_KATP

Rule I_KATP is an assignment rule for parameter I_KATP:

$$\text{I\_KATP} = \text{gmkatp} \cdot \text{Okatp} \cdot (\text{V} - \text{Vk}) \tag{32}$$

Derived unit $\text{pS} \cdot \text{mV}$

6.33 Rule Jerp

Rule Jerp is an assignment rule for parameter Jerp:

$$\text{Jerp} = \frac{\text{Pcaer} \cdot [\text{Ca\_cyt}]^2}{[\text{Ca\_cyt}]^2 + \text{Kcarp}^2} \tag{33}$$

Derived unit $1.0000000000000024 \cdot 10^{-6}\ \text{mol} \cdot \text{ms}^{-1} \cdot \text{l}^{-1}$

6.34 Rule O_infinity

Rule O_infinity is an assignment rule for parameter O_infinity:

$$\text{O\_infinity} = \frac{[\text{Ca\_cyt}] \cdot [\text{IP3\_cyt}]^3}{([\text{Ca\_cyt}] + \text{Krca}) \cdot \left([\text{IP3\_cyt}]^3 + \text{Kip3}^3\right)} \tag{34}$$

Derived unit dimensionless

6.35 Rule Jout

Rule Jout is an assignment rule for parameter Jout:

$$\text{Jout} = (\text{Pleak} + \text{Pip3} \cdot \text{O\_infinity}) \cdot ([\text{Ca\_er}] - [\text{Ca\_cyt}]) \tag{35}$$

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

6.36 Rule n

Rule n is a rate rule for parameter n:

$$\frac{\text{d}}{\text{d}t}\text{n} = \frac{\text{n\_infinity} - \text{n}}{\text{tau\_n}} \tag{36}$$

6.37 Rule V

Rule V is a rate rule for parameter V:

$$\begin{aligned} &\frac{\text{d}}{\text{d}t}\text{V} \\ &= \frac{0 - (\text{I\_Vca} + \text{I\_CaPump} + \text{I\_NaCa} + \text{I\_CRAN} + \text{I\_Na} + \text{I\_NaK} + \text{I\_KDr} + \text{I\_KCa} + \text{I\_KATP})}{\text{Cm}} \end{aligned} \tag{37}$$

7 Reactions

This model contains 18 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	Calcium_cyt_Ivca		$\emptyset \longrightarrow$ Ca_cyt	
2	Calcium_cyt_Inaca		$\emptyset \longrightarrow$ Ca_cyt	
3	Calcium_cyt_Icapump		Ca_cyt $\longrightarrow \emptyset$	
4	Calcium_cyt_Jerp		$0 \cdot 01$ Ca_cyt $\longrightarrow 0 \cdot 03$ Ca_er	
5	Calcium_cyt_Jout		$0 \cdot 03$ Ca_er $\longrightarrow 0 \cdot 01$ Ca_cyt	
6	Calcium_cyt_sequestration		Ca_cyt $\longrightarrow \emptyset$	
7	IP3_synthesis		$\emptyset \xrightarrow{\text{Ca\_cyt}}$ IP3_cyt	
8	IP3_degradation		IP3_cyt $\longrightarrow \emptyset$	
9	Na_Inaca		Na_cyt $\longrightarrow \emptyset$	
10	Na_Inak		Na_cyt $\longrightarrow \emptyset$	
11	Na_Ina		$\emptyset \longrightarrow$ Na_cyt	
12	Na_Icran		$\emptyset \longrightarrow$ Na_cyt	
13	ATP_production		$\emptyset \xrightarrow{\text{ADP\_cyt}}$ ATP_cyt	
14	ATP_NaKATPase		ATP_cyt $\longrightarrow \emptyset$	
15	ATP_Capump		ATP_cyt $\longrightarrow \emptyset$	
16	ATP_Jerp		ATP_cyt $\longrightarrow \emptyset$	

№	Id	Name	Reaction Equation	SBO
17	ATP_Ca-_dependent-_consumption		$\text{ATP\_cyt} \xrightarrow{\text{Ca\_cyt}} \emptyset$	
18	ATP_consumption		$\text{ATP\_cyt} \longrightarrow \emptyset$	

7.1 Reaction Calcium_cyt_Ivca

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

Reaction equation

$$\emptyset \longrightarrow \text{Ca\_cyt} \tag{38}$$

Product

Table 6: Properties of each product.

Id	Name	SBO
Ca_cyt	Cytosolic Calcium	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \frac{\text{fi} \cdot (\text{I\_Vca})}{2 \cdot \text{F}} \tag{39}$$

7.2 Reaction Calcium_cyt_Inaca

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

Reaction equation

$$\emptyset \longrightarrow \text{Ca\_cyt} \tag{40}$$

Product

Table 7: Properties of each product.

Id	Name	SBO
Ca_cyt	Cytosolic Calcium	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \frac{\text{fi} \cdot 2 \cdot \text{I\_NaCa}}{2 \cdot \text{F}} \tag{41}$$

7.3 Reaction `Calcium_cyt_Icapump`

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

Reaction equation

$$\text{Ca\_cyt} \longrightarrow \emptyset \tag{42}$$

Reactant

Table 8: Properties of each reactant.

Id	Name	SBO
`Ca_cyt`	Cytosolic Calcium	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \frac{\text{fi} \cdot 2 \cdot \text{I\_CaPump}}{2 \cdot \text{F}} \tag{43}$$

7.4 Reaction `Calcium_cyt_Jerp`

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

Reaction equation

$$0{\cdot}01\,\text{Ca\_cyt} \longrightarrow 0{\cdot}03\,\text{Ca\_er} \tag{44}$$

Reactant

Table 9: Properties of each reactant.

Id	Name	SBO
`Ca_cyt`	Cytosolic Calcium	

Product

Table 10: Properties of each product.

Id	Name	SBO
`Ca_er`	ER Calcium	

Id	Name	SBO

Kinetic Law

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

$$v_4 = \text{vol}(\text{Cytoplasm}) \cdot \text{Jerp} \tag{45}$$

7.5 Reaction `Calcium_cyt_Jout`

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

Reaction equation

$$0{\cdot}03\,\text{Ca\_er} \longrightarrow 0{\cdot}01\,\text{Ca\_cyt} \tag{46}$$

Reactant

Table 11: Properties of each reactant.

Id	Name	SBO
`Ca_er`	ER Calcium	

Product

Table 12: Properties of each product.

Id	Name	SBO
`Ca_cyt`	Cytosolic Calcium	

Kinetic Law

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

$$v_5 = \text{Jout} \tag{47}$$

7.6 Reaction `Calcium_cyt_sequestration`

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

Reaction equation

$$\text{Ca\_cyt} \longrightarrow \emptyset \tag{48}$$

Reactant

Table 13: Properties of each reactant.

Id	Name	SBO
Ca_cyt	Cytosolic Calcium	

Kinetic Law

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

$$v_6 = \mathrm{vol}\,(\mathrm{Cytoplasm}) \cdot \mathrm{ksg} \cdot [\mathrm{Ca\_cyt}] \tag{49}$$

7.7 Reaction IP3_synthesis

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

Reaction equation

$$\emptyset \xrightarrow{\mathrm{Ca\_cyt}} \mathrm{IP3\_cyt} \tag{50}$$

Modifier

Table 14: Properties of each modifier.

Id	Name	SBO
Ca_cyt	Cytosolic Calcium	

Product

Table 15: Properties of each product.

Id	Name	SBO
IP3_cyt	Cytosolic IP3	

Kinetic Law

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

$$v_7 = \frac{\mathrm{vol}\,(\mathrm{Cytoplasm}) \cdot \mathrm{kip} \cdot [\mathrm{Ca\_cyt}]^2}{[\mathrm{Ca\_cyt}]^2 + \mathrm{Kipca}^2} \tag{51}$$

7.8 Reaction IP3_degradation

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

Reaction equation

$$\text{IP3\_cyt} \longrightarrow \emptyset \tag{52}$$

Reactant

Table 16: Properties of each reactant.

Id	Name	SBO
IP3_cyt	Cytosolic IP3	

Kinetic Law

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

$$v_8 = \text{vol}\,(\text{Cytoplasm}) \cdot \text{kdip} \cdot [\text{IP3\_cyt}] \tag{53}$$

7.9 Reaction Na_Inaca

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

Reaction equation

$$\text{Na\_cyt} \longrightarrow \emptyset \tag{54}$$

Reactant

Table 17: Properties of each reactant.

Id	Name	SBO
Na_cyt	Cytosolic Sodium	

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \frac{3 \cdot \text{I\_NaCa}}{\text{F}} \tag{55}$$

7.10 Reaction Na_Inak

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

Reaction equation

$$\text{Na\_cyt} \longrightarrow \emptyset \tag{56}$$

Reactant

Table 18: Properties of each reactant.

Id	Name	SBO
Na_cyt	Cytosolic Sodium	

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = \frac{3 \cdot \text{I\_NaK}}{\text{F}} \tag{57}$$

7.11 Reaction Na_Ina

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

Reaction equation

$$\emptyset \longrightarrow \text{Na\_cyt} \tag{58}$$

Product

Table 19: Properties of each product.

Id	Name	SBO
Na_cyt	Cytosolic Sodium	

Kinetic Law

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

$$v_{11} = \frac{\text{I\_Na}}{\text{F}} \tag{59}$$

7.12 Reaction Na_Icran

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

Reaction equation

$$\emptyset \longrightarrow \text{Na\_cyt} \tag{60}$$

Product

Table 20: Properties of each product.

Id	Name	SBO
Na_cyt	Cytosolic Sodium	

Kinetic Law

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

$$v_{12} = \frac{\text{I\_CRAN}}{\text{F}} \tag{61}$$

7.13 Reaction ATP_production

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

Reaction equation

$$\emptyset \xrightarrow{\text{ADP\_cyt}} \text{ATP\_cyt} \tag{62}$$

Modifier

Table 21: Properties of each modifier.

Id	Name	SBO
ADP_cyt	Cytosolic ADP	

Product

Table 22: Properties of each product.

Id	Name	SBO
ATP_cyt	Cytosolic ATP	

Kinetic Law

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

$$v_{13} = \mathrm{vol}\,(\mathrm{Cytoplasm}) \cdot \mathrm{kadp} \cdot [\mathrm{ADP\_cyt}] \tag{63}$$

7.14 Reaction ATP_NaKATPase

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

Reaction equation

$$\mathrm{ATP\_cyt} \longrightarrow \emptyset \tag{64}$$

Reactant

Table 23: Properties of each reactant.

Id	Name	SBO
ATP_cyt	Cytosolic ATP	

Kinetic Law

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

$$v_{14} = \frac{\mathrm{I\_NaK}}{\mathrm{F}} \tag{65}$$

7.15 Reaction ATP_Capump

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

Reaction equation

$$\mathrm{ATP\_cyt} \longrightarrow \emptyset \tag{66}$$

Reactant

Table 24: Properties of each reactant.

Id	Name	SBO
ATP_cyt	Cytosolic ATP	

Kinetic Law

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

$$v_{15} = \frac{\mathrm{I\_CaPump}}{\mathrm{F}} \tag{67}$$

7.16 Reaction ATP_Jerp

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

Reaction equation

$$\mathrm{ATP\_cyt} \longrightarrow \emptyset \tag{68}$$

Reactant

Table 25: Properties of each reactant.

Id	Name	SBO
ATP_cyt	Cytosolic ATP	

Kinetic Law

Derived unit contains undeclared units

$$v_{16} = \frac{\mathrm{vol}\,(\mathrm{Cytoplasm}) \cdot \mathrm{Jerp}}{2} \tag{69}$$

7.17 Reaction ATP_Ca_dependent_consumption

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

Reaction equation

$$\mathrm{ATP\_cyt} \xrightarrow{\mathrm{Ca\_cyt}} \emptyset \tag{70}$$

Reactant

Table 26: Properties of each reactant.

Id	Name	SBO
ATP_cyt	Cytosolic ATP	

Modifier

Table 27: Properties of each modifier.

Id	Name	SBO
Ca_cyt	Cytosolic Calcium	

Kinetic Law

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

$$v_{17} = \mathrm{vol}\,(\mathrm{Cytoplasm}) \cdot \mathrm{katpca} \cdot [\mathrm{Ca\_cyt}] \cdot [\mathrm{ATP\_cyt}] \tag{71}$$

7.18 Reaction ATP_consumption

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

Reaction equation

$$\mathrm{ATP\_cyt} \longrightarrow \emptyset \tag{72}$$

Reactant

Table 28: Properties of each reactant.

Id	Name	SBO
ATP_cyt	Cytosolic ATP	

Kinetic Law

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

$$v_{18} = \mathrm{vol}\,(\mathrm{Cytoplasm}) \cdot \mathrm{katp} \cdot [\mathrm{ATP\_cyt}] \tag{73}$$

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

Name Cytosolic Calcium

Initial concentration $0.085\ \mu\text{mol}\cdot\text{l}^{-1}$

This species takes part in eight reactions (as a reactant in Calcium_cyt_Icapump, Calcium_cyt_Jerp, Calcium_cyt_sequestration and as a product in Calcium_cyt_Ivca, Calcium_cyt_Inaca, Calcium_cyt_Jout and as a modifier in IP3_synthesis, ATP_Ca_dependent_consumption).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Ca\_cyt} = v_1 + v_2 + 0.01v_5 - v_3 - 0.01v_4 - v_6 \tag{74}$$

8.2 Species Ca_er

Name ER Calcium

Initial concentration $22.8\ \mu\text{mol}\cdot\text{l}^{-1}$

This species takes part in two reactions (as a reactant in Calcium_cyt_Jout and as a product in Calcium_cyt_Jerp).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Ca\_er} = 0.03v_4 - 0.03v_5 \tag{75}$$

8.3 Species IP3_cyt

Name Cytosolic IP3

Initial concentration $0.33\ \mu\text{mol}\cdot\text{l}^{-1}$

This species takes part in two reactions (as a reactant in IP3_degradation and as a product in IP3_synthesis).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{IP3\_cyt} = v_7 - v_8 \tag{76}$$

8.4 Species Na_cyt

Name Cytosolic Sodium

Initial concentration 9858 $\mu mol \cdot l^{-1}$

This species takes part in four reactions (as a reactant in Na_Inaca, Na_Inak and as a product in Na_Ina, Na_Icran).

$$\frac{d}{dt}\text{Na\_cyt} = v_{11} + v_{12} - v_9 - v_{10} \tag{77}$$

8.5 Species ATP_cyt

Name Cytosolic ATP

Initial concentration 932.1 $\mu mol \cdot l^{-1}$

This species takes part in six reactions (as a reactant in ATP_NaKATPase, ATP_Capump, ATP_Jerp, ATP_Ca_dependent_consumption, ATP_consumption and as a product in ATP_production).

$$\frac{d}{dt}\text{ATP\_cyt} = v_{13} - v_{14} - v_{15} - v_{16} - v_{17} - v_{18} \tag{78}$$

8.6 Species ADP_cyt

Name Cytosolic ADP

Initial concentration 3067.9 $\mu mol \cdot l^{-1}$

Involved in rule ADP_cyt

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

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