SBML Model Report

Model name: "Clancy2001_Kchannel"

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1 General Overview

This is a document in SBML Level 2 Version 1 format. This model was created by Enuo He[1] at June 20th 2007 at 9:51 a. m. and last time modified at October tenth 2014 at 10:18 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	1
species types	0	species	6
events	2	constraints	0
reactions	5	function definitions	0
global parameters	19	unit definitions	3
rules	10	initial assignments	0

Model Notes

This model is according to the paper *Cellular consequences of HEGR mutations in the long QT syndrome: precursors to sudden cardiac death.* The author used Markovian model of cardiac Ikr in the paper. Figure4B in the paper has been reproduced using CellDesigner3.5.1. The cell is depolarized to the indicated test potential for 250ms (from 50ms to 300ms) from a holding potential of -40mV and then repolarized to -40mV. Change the value for vtest from -30,-20,-10,0,10,20,30,40 for each simulation in order to produce the different cureve in the paper.

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

2.1 Unit `time`

Name ms

Definition ms

2.2 Unit `mV`

Definition mV

2.3 Unit `substance`

Name mM

Definition mmol

2.4 Unit `volume`

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

Definition l

2.5 Unit `area`

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

Definition m^2

2.6 Unit `length`

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

Definition m

3 Compartment

This model contains one compartment.

Table 2: Properties of all compartments.

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

3.1 Compartment `cell`

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

4 Species

This model contains six species. Section 9 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
c3	ClosedState_3	cell	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
c2	ClosedState_2	cell	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
c1	ClosedState_1	cell	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
o	OpenState	cell	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
i	InactivationState	cell	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
ik	cardiac delayed rectifier current	cell	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟

5 Parameters

This model contains 19 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
R	gas constant		8.314		☑
F	Faraday constant		96.485		☑
Temp	temperature		310.000		☑
ko	extracellular K		5.400		☑
ki	introcellular K		140.000		☑
vhold	holding_potential		−40.000		☑
vtest	test_potential		0.000		☑
vk	reversal potential for k		0.000		⊟
Gk	membrane-_conductance		0.000		⊟
a			0.000		⊟
b			0.000		⊟
ain			2.172		☑
bin			1.077		☑
aa			0.000		⊟
bb			0.000		⊟
ai			0.000		⊟
bi			0.000		⊟
u			0.000		⊟
v	membrane-_potential		−40.000		⊟

6 Rules

This is an overview of ten rules.

6.1 Rule vk

Rule vk is an assignment rule for parameter vk:

$$\mathrm{vk} = \frac{\mathrm{R} \cdot \mathrm{Temp}}{\mathrm{F}} \cdot \left(\frac{\mathrm{ko}}{\mathrm{ki}} \right) \tag{1}$$

6.2 Rule Gk

Rule Gk is an assignment rule for parameter Gk:

$$\mathrm{Gk} = 0.013500000000000002 \cdot \mathrm{ko}^{0.59} \tag{2}$$

6.3 Rule a

Rule a is an assignment rule for parameter a:

$$\mathrm{a} = 0.0555 \cdot \exp(0.05547153 \cdot (\mathrm{v} - 12)) \tag{3}$$

6.4 Rule b

Rule b is an assignment rule for parameter b:

$$\mathrm{b} = 0.002357 \cdot \exp(-0.036588 \cdot \mathrm{v}) \tag{4}$$

6.5 Rule aa

Rule aa is an assignment rule for parameter aa:

$$\mathrm{aa} = 0.0655 \cdot \exp(0.05547153 \cdot (\mathrm{v} - 36)) \tag{5}$$

6.6 Rule bb

Rule bb is an assignment rule for parameter bb:

$$\mathrm{bb} = 0.0029357000000000003 \cdot \exp(-0.02158 \cdot \mathrm{v}) \tag{6}$$

6.7 Rule ai

Rule ai is an assignment rule for parameter ai:

$$\mathrm{ai} = \frac{0.439 \cdot \exp(-0.02352 \cdot (\mathrm{v} + 25)) \cdot 4.5}{\mathrm{ko}} \tag{7}$$

6.8 Rule bi

Rule bi is an assignment rule for parameter bi:

$$\mathrm{bi} = 0.656 \cdot \exp(9.42 \cdot 10^{-4} \cdot \mathrm{v} \cdot \left(\tfrac{4.5}{\mathrm{ko}}\right)^{0.3} \tag{8}$$

6.9 Rule u

Rule u is an assignment rule for parameter u:

$$\mathrm{u} = \frac{\mathrm{ai} \cdot \mathrm{bb} \cdot \mathrm{aa}}{\mathrm{aa} \cdot \mathrm{bi}} \tag{9}$$

6.10 Rule ik

Rule ik is an assignment rule for species ik:

$$\mathrm{ik} = \mathrm{Gk} \cdot [\mathrm{o}] \cdot (\mathrm{v} - \mathrm{vk}) \tag{10}$$

7 Events

This is an overview of two events. Each event is initiated whenever its trigger condition switches from false to true. A delay function postpones the effects of an event to a later time point. At the time of execution, an event can assign values to species, parameters or compartments if these are not set to constant.

7.1 Event event_0000001

Notes when (t gt 50) and (t lt 300), v=vtest

Trigger condition

$$(\mathrm{time} > 50) \wedge (\mathrm{time} \leq 300) \tag{11}$$

Assignment

$$\mathrm{v} = \mathrm{vtest} \tag{12}$$

7.2 Event event_0000002

Notes when t > 300, v=vhold.

Trigger condition

$$\mathrm{time} > 300 \tag{13}$$

Assignment

$$\mathrm{v} = \mathrm{vhold} \tag{14}$$

8 Reactions

This model contains five 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	reaction_0000001	c3-c2 transition	c3 $\rightleftharpoons$ c2	
2	reaction_0000002	c2-c1 transition	c2 $\rightleftharpoons$ c1	
3	reaction_0000003	c1-o transition	c1 $\rightleftharpoons$ o	
4	reaction_0000004	o-i transition	o $\rightleftharpoons$ i	
5	reaction_0000005	c1-i transition	c1 $\rightleftharpoons$ i	

8.1 Reaction reaction_0000001

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

Name c3-c2 transition

Reaction equation

$$\mathrm{c3} \rightleftharpoons \mathrm{c2} \tag{15}$$

Reactant

Table 6: Properties of each reactant.

Id	Name	SBO
c3	ClosedState_3	

Product

Table 7: Properties of each product.

Id	Name	SBO
c2	ClosedState_2	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = (\mathrm{a} \cdot [\mathrm{c3}] - \mathrm{b} \cdot [\mathrm{c2}]) \cdot \mathrm{vol}\,(\mathrm{cell}) \tag{16}$$

8.2 Reaction reaction_0000002

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

Name c2-c1 transition

Reaction equation

$$\mathrm{c2} \rightleftharpoons \mathrm{c1} \tag{17}$$

Reactant

Table 8: Properties of each reactant.

Id	Name	SBO
c2	ClosedState_2	

Product

Table 9: Properties of each product.

Id	Name	SBO
c1	ClosedState_1	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = (\mathrm{ain} \cdot [\mathrm{c2}] - \mathrm{bin} \cdot [\mathrm{c1}]) \cdot \mathrm{vol}\,(\mathrm{cell}) \tag{18}$$

8.3 Reaction reaction_0000003

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

Name c1-o transition

Reaction equation

$$\mathrm{c1} \rightleftharpoons \mathrm{o} \tag{19}$$

Reactant

Table 10: Properties of each reactant.

Id	Name	SBO
c1	ClosedState_1	

Product

Table 11: Properties of each product.

Id	Name	SBO
o	OpenState	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = ([\mathrm{c1}] \cdot \mathrm{aa} - \mathrm{bb} \cdot [\mathrm{o}]) \cdot \mathrm{vol}(\mathrm{cell}) \tag{20}$$

8.4 Reaction `reaction_0000004`

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

Name o-i transition

Reaction equation

$$\mathrm{o} \rightleftharpoons \mathrm{i} \tag{21}$$

Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
o	OpenState	

Product

Table 13: Properties of each product.

Id	Name	SBO
i	InactivationState	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = ([\mathrm{o}] \cdot \mathrm{bi} - \mathrm{ai} \cdot [\mathrm{i}]) \cdot \mathrm{vol}(\mathrm{cell}) \tag{22}$$

8.5 Reaction `reaction_0000005`

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

Name c1-i transition

Reaction equation

$$\mathrm{c1} \rightleftharpoons \mathrm{i} \tag{23}$$

Reactant

Table 14: Properties of each reactant.

Id	Name	SBO
c1	ClosedState_1	

Product

Table 15: Properties of each product.

Id	Name	SBO
i	InactivationState	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = (\mathrm{aa} \cdot [\mathrm{c1}] - \mathrm{u} \cdot [\mathrm{i}]) \cdot \mathrm{vol}\,(\mathrm{cell}) \tag{24}$$

9 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.

9.1 Species c3

Name ClosedState_3

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

This species takes part in one reaction (as a reactant in reaction_0000001).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{c3} = -\,v_1 \tag{25}$$

9.2 Species c2

Name ClosedState_2

Initial concentration $0\ \mathrm{mmol} \cdot \mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in reaction_0000002 and as a product in reaction_0000001).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{c2} = v_1 - v_2 \tag{26}$$

9.3 Species c1

Name ClosedState_1

Initial concentration $0\ \mathrm{mmol} \cdot \mathrm{l}^{-1}$

This species takes part in three reactions (as a reactant in reaction_0000003, reaction_0000005 and as a product in reaction_0000002).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{c1} = v_2 - v_3 - v_5 \tag{27}$$

9.4 Species o

Name OpenState

Initial concentration $0.06\ \mathrm{mmol} \cdot \mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in reaction_0000004 and as a product in reaction_0000003).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{o} = v_3 - v_4 \tag{28}$$

9.5 Species i

Name InactivationState

Initial concentration $0\ \mathrm{mmol} \cdot \mathrm{l}^{-1}$

This species takes part in two reactions (as a product in reaction_0000004, reaction_0000005).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{i} = v_4 + v_5 \tag{29}$$

9.6 Species ik

Name cardiac delayed rectifier current

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

Involved in rule ik

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.

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