SBML Model Report

Model name: “Zhu2007_TF_modulated_by_Calcium”

May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by Harish Dharuri[1] at December 21st 2007 at 9:55 a. m. and last time modified at May 27th 2014 at 10:02 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	9	function definitions	0
global parameters	7	unit definitions	2
rules	2	initial assignments	0

Model Notes

This a model from the article:
A theoretical study on activation of transcription factor modulated by intracellular Ca2+ oscillations.
Zhu CL, Zheng Y, Jia Y Biophys. Chem.[2007 Aug:129(1):49-55 17560007,

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Abstract:
This work presents both deterministic and stochastic models of genetic expression modulated by intracellular calcium (Ca2+) oscillations, based on macroscopic differential equations and chemical Langevin equations, respectively. In deterministic case, the oscillations of intracellular Ca2+ decrease the effective Ca2+ threshold for the activation of transcriptional activator (TF-A). The average activation of TF-A increases with the increase of the average amplitude of intracellular Ca2+ oscillations, but decreases with the increase of the period of intracellular Ca2+ oscillations, which are qualitatively consistent with the experimental results on the gene expression in lymphocytes. In stochastic case, it is found that a large internal fluctuation of the biochemical reaction can enhance gene expression efficiency specifically at a low level of external stimulations or at a small rate of TF-A dimer phosphorylation activated by Ca2+, which reduces the threshold of the average intracellular Ca2+ concentration for gene expression.

2 Unit Definitions

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

2.1 Unit substance

Name micro mole

Definition µmol

2.2 Unit time

Name minutes

Definition 60 s

2.3 Unit volume

Notes Litre is the predefined SBML unit for volume.

Definition l

2.4 Unit `area`

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

Definition m^2

2.5 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	1	litre	☑	
`store`	store		3	1	litre	☑	

3.1 Compartment `cytoplasm`

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

Name cytoplasm

3.2 Compartment `store`

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

Name store

4 Species

This model contains three 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
X	TF_A	cytoplasm	$\mu mol \cdot l^{-1}$	⊟	⊟
Y	Calcium in store	store	$\mu mol \cdot l^{-1}$	⊟	⊟
Z	Calcium in cytoplasm	cytoplasm	$\mu mol \cdot l^{-1}$	⊟	⊟

5 Parameters

This model contains seven global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
kf	kf		0.0		☐
Kd	Kd		0.0		☐
kf0			6.0		☑
gamma			9.0		☑
Ka	Ka		0.5		☑
Kb	Kb		0.5		☑
Kd0			10.0		☑

6 Rules

This is an overview of two rules.

6.1 Rule kf

Rule kf is an assignment rule for parameter kf:

$$\mathrm{kf} = \mathrm{kf0} \cdot \left(1 + \frac{\mathrm{gamma} \cdot [\mathrm{Z}]^4}{\mathrm{Ka}^4 + [\mathrm{Z}]^4}\right) \tag{1}$$

6.2 Rule Kd

Rule Kd is an assignment rule for parameter Kd:

$$\mathrm{Kd} = \frac{\mathrm{Kd0}}{1 + \frac{[\mathrm{Z}]^4}{\mathrm{Kb}^4}} \tag{2}$$

7 Reactions

This model contains nine 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	`TF_synthesis`	TF Synthesis	$\emptyset \rightleftharpoons X$	
2	`TF_degradation`	TF degradation	$X \rightleftharpoons \emptyset$	
3	`TF_synthesis_basal`	TF_synthesis_basal	$\emptyset \rightleftharpoons X$	
4	`Calcium_Influx`	Calcium_Influx	$\emptyset \rightleftharpoons Z$	
5	`Calcium_Influx_stimulation`	Calcium Influx by stimulation	$\emptyset \rightleftharpoons Z$	
6	`Calcium_into_store`	Calcium Influx	$Z \rightleftharpoons Y$	
7	`Calcium_into_cytoplasm`	Calcium influx to cytoplasm	$Y \rightleftharpoons Z$	
8	`Leakage`	Calcium Leakage	$Y \rightleftharpoons Z$	
9	`Leakage_from_cytoplasm`	Leakage from cytoplasm	$Z \rightleftharpoons \emptyset$	

7.1 Reaction TF_synthesis

This is a reversible reaction of no reactant forming one product.

Name TF Synthesis

Reaction equation

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

Product

Table 6: Properties of each product.

Id	Name	SBO
X	TF_A	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \frac{\mathrm{kf} \cdot [\mathrm{X}]^2}{[\mathrm{X}]^2 + \mathrm{Kd}} \tag{4}$$

7.2 Reaction TF_degradation

This is a reversible reaction of one reactant forming no product.

Name TF degradation

Reaction equation

$$\mathrm{X} \rightleftharpoons \emptyset \tag{5}$$

Reactant

Table 7: Properties of each reactant.

Id	Name	SBO
X	TF_A	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \mathrm{kd} \cdot [\mathrm{X}] \tag{6}$$

Table 8: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
kd			1.0		☑

7.3 Reaction TF_synthesis_basal

This is a reversible reaction of no reactant forming one product.

Name TF_synthesis_basal

Reaction equation

$$\emptyset \rightleftharpoons \mathrm{X} \tag{7}$$

Product

Table 9: Properties of each product.

Id	Name	SBO
X	TF_A	

Kinetic Law

Derived unit not available

$$v_3 = \mathrm{Rbas} \tag{8}$$

Table 10: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Rbas	Rbas		0.1		☑

7.4 Reaction Calcium_Influx

This is a reversible reaction of no reactant forming one product.

Name Calcium_Influx

Reaction equation

$$\emptyset \rightleftharpoons Z \tag{9}$$

Product

Table 11: Properties of each product.

Id	Name	SBO
Z	Calcium in cytoplasm	

Kinetic Law

Derived unit not available

$$v_4 = \mathrm{v0} \tag{10}$$

Table 12: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
v0			1.0		☑

7.5 Reaction `Calcium_Influx_stimulation`

This is a reversible reaction of no reactant forming one product.

Name Calcium Influx by stimulation

Reaction equation

$$\emptyset \rightleftharpoons Z \tag{11}$$

Product

Table 13: Properties of each product.

Id	Name	SBO
Z	Calcium in cytoplasm	

Kinetic Law

Derived unit not available

$$v_5 = \mathrm{v1} \cdot \mathrm{beta} \tag{12}$$

Table 14: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
v1			5.7		☑
beta			0.3		☑

7.6 Reaction Calcium_into_store

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

Name Calcium Influx

Reaction equation

$$\mathrm{Z} \rightleftharpoons \mathrm{Y} \tag{13}$$

Reactant

Table 15: Properties of each reactant.

Id	Name	SBO
Z	Calcium in cytoplasm	

Product

Table 16: Properties of each product.

Id	Name	SBO
Y	Calcium in store	

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \frac{\mathrm{Vm2} \cdot [\mathrm{Z}]^{\mathrm{n}}}{\mathrm{K2}^{\mathrm{n}} + [\mathrm{Z}]^{\mathrm{n}}} \tag{14}$$

Table 17: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vm2			30.0		☑
K2			0.5		☑
n			2.0		☑

7.7 Reaction Calcium_into_cytoplasm

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

Name Calcium influx to cytoplasm

Reaction equation

$$\mathrm{Y} \rightleftharpoons \mathrm{Z} \tag{15}$$

Reactant

Table 18: Properties of each reactant.

Id	Name	SBO
Y	Calcium in store	

Product

Table 19: Properties of each product.

Id	Name	SBO
Z	Calcium in cytoplasm	

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \frac{\frac{\mathrm{Vm3} \cdot [\mathrm{Y}]^{\mathrm{m}}}{\mathrm{Kr}^{\mathrm{m}} + [\mathrm{Y}]^{\mathrm{m}}} \cdot [\mathrm{Z}]^{\mathrm{p}}}{\mathrm{K\_A}^{\mathrm{p}} + [\mathrm{Z}]^{\mathrm{p}}} \tag{16}$$

Table 20: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vm3			325.00		☑
Kr			1.70		☑
K_A			0.46		☑
m			2.00		☑
p			4.00		☑

7.8 Reaction Leakage

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

Name Calcium Leakage

Reaction equation

$$\mathrm{Y} \rightleftharpoons \mathrm{Z} \tag{17}$$

Reactant

Table 21: Properties of each reactant.

Id	Name	SBO
Y	Calcium in store	

Product

Table 22: Properties of each product.

Id	Name	SBO
Z	Calcium in cytoplasm	

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \mathrm{k1} \cdot [\mathrm{Y}] \tag{18}$$

Table 23: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1			0.7		☑

7.9 Reaction Leakage_from_cytoplasm

This is a reversible reaction of one reactant forming no product.

Name Leakage from cytoplasm

Reaction equation

$$Z \rightleftharpoons \emptyset \tag{19}$$

Reactant

Table 24: Properties of each reactant.

Id	Name	SBO
Z	Calcium in cytoplasm	

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \mathrm{k} \cdot [\mathrm{Z}] \tag{20}$$

Table 25: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k			10.0		☑

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.

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.

8.1 Species X

Name TF_A

Initial concentration $15\ \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in three reactions (as a reactant in TF_degradation and as a product in TF_synthesis, TF_synthesis_basal).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{X} = v_1 + v_3 - v_2 \tag{21}$$

8.2 Species Y

Name Calcium in store

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

This species takes part in three reactions (as a reactant in Calcium_into_cytoplasm, Leakage and as a product in Calcium_into_store).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Y} = v_6 - v_7 - v_8 \tag{22}$$

8.3 Species Z

Name Calcium in cytoplasm

Initial concentration $0.25\ \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in six reactions (as a reactant in Calcium_into_store, Leakage_from_cytoplasm and as a product in Calcium_Influx, Calcium_Influx_stimulation, Calcium_into_cytoplasm, Leakage).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Z} = v_4 + v_5 + v_7 + v_8 - v_6 - v_9 \tag{23}$$

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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