SBML Model Report

Model name: "Rozi2003-_GlycogenPhosphorylase_Activation"

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 March 22nd 2007 at 10:28 a. m. and last time modified at May 24th 2014 at 5:51 p. m. Table 1 gives 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	5
events	0	constraints	0
reactions	10	function definitions	0
global parameters	30	unit definitions	5
rules	0	initial assignments	0

Model Notes

The model reproduces the temporal evolution of Glycogen phosphorylase for a vale of Vm5=30 as depicted in Fig 1a of the paper. The model makes use of calcium oscillations from the Borghans model to stimulate the activation of glycogen phosphorylase. Hence, this is a simple extension of the Borghans model. The model was succesfully tested on MathSBML and Jarnac.

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2 Unit Definitions

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

2.1 Unit `substance`

Name micromole

Definition $\mu\mathrm{mol}$

2.2 Unit `uM`

Name uM

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

2.3 Unit `uM_per_min`

Name uM_per_min

Definition $\mu\mathrm{mol} \cdot \mathrm{l}^{-1} \cdot (3600\ \mathrm{s})^{-1}$

2.4 Unit `time`

Name minutes

Definition $3600\ \mathrm{s}$

2.5 Unit `min_inv`

Name min_inv

Definition $(3600\ \mathrm{s})^{-1}$

2.6 Unit volume

Notes Litre is the predefined SBML unit for volume.

Definition l

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

3 Compartments

This model contains three compartments.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
extracellular			3	1	litre	☑	
cytosol			3	1	litre	☑	extracellular
intravesicular			3	1	litre	☑	cytosol

3.1 Compartment extracellular

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

3.2 Compartment cytosol

This is a three dimensional compartment with a constant size of one litre, which is surrounded by extracellular.

3.3 Compartment intravesicular

This is a three dimensional compartment with a constant size of one litre, which is surrounded by cytosol.

4 Species

This model contains five species. The boundary condition of one of these species is set to `true` so that this species' amount cannot be changed by any reaction. 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
`EC`	Extracellular Calcium	`extracellular`	$\mu mol \cdot l^{-1}$	⊟	☑
`Z`	Cytosolic Calcium	`cytosol`	$\mu mol \cdot l^{-1}$	⊟	⊟
`A`	IP3	`cytosol`	$\mu mol \cdot l^{-1}$	⊟	⊟
`Y`	Intravesicular Calcium	`intravesicular`	$\mu mol \cdot l^{-1}$	⊟	⊟
`GP`	Glycogen Phosphorylase	`cytosol`	$\mu mol \cdot l^{-1}$	⊟	⊟

5 Parameters

This model contains 30 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
v0			2.0	$\mu mol \cdot l^{-1} \cdot (3600\ s)^{-1}$	☑
v1			2.0	$\mu mol \cdot l^{-1} \cdot (3600\ s)^{-1}$	☑
beta			0.5	dimensionless	☑
Vm2			6.0	$\mu mol \cdot l^{-1} \cdot (3600\ s)^{-1}$	☑
K2			0.1	$\mu mol \cdot l^{-1}$	☑
Vm3			20.0	$\mu mol \cdot l^{-1} \cdot (3600\ s)^{-1}$	☑
m			2.0	dimensionless	☑
Ka			0.2	$\mu mol \cdot l^{-1}$	☑
Ky			0.2	$\mu mol \cdot l^{-1}$	☑
Kz			0.5	$\mu mol \cdot l^{-1}$	☑
Kf			1.0	$(3600\ s)^{-1}$	☑
K			10.0	$(3600\ s)^{-1}$	☑
V4			2.0	$\mu mol \cdot l^{-1} \cdot (3600\ s)^{-1}$	☑
Vm5			30.0	$\mu mol \cdot l^{-1} \cdot (3600\ s)^{-1}$	☑
n			4.0	dimensionless	☑
K5			1.0	$\mu mol \cdot l^{-1}$	☑
Kd			0.4	$\mu mol \cdot l^{-1}$	☑
epsilon			0.1	$(3600\ s)^{-1}$	☑
Vpm1			1.5	$(3600\ s)^{-1}$	☑
gamma			9.0	dimensionless	☑
Ka5			0.5	$\mu mol \cdot l^{-1}$	☑
K1			0.1		☑
Ka6			0.5	$\mu mol \cdot l^{-1}$	☑
Vpm2			0.6	$(3600\ s)^{-1}$	☑
alpha			9.0	dimensionless	☑
G			10000.0	$\mu mol \cdot l^{-1}$	☑
Ka1			10000.0	$\mu mol \cdot l^{-1}$	☑
Kp2			0.2		☑
Ka2			10000.0	$\mu mol \cdot l^{-1}$	☑
p			2.0	dimensionless	☑

6 Reactions

This model contains ten 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	vin	Calcium Influx	$EC \longrightarrow Z$	
2	R2	Calcium transport to internal store	$Z \longrightarrow Y$	
3	R3	Calcium transport to cytosol	$Y \xrightarrow{A} Z$	
4	Rkf	Calcium leak	$Y \longrightarrow Z$	
5	Rkz	Calcium efflux	$Z \longrightarrow EC$	
6	R4	Agonist stimulated production of IP3	$\emptyset \longrightarrow A$	
7	R5	Ca-dependant IP3 degradation	$A \xrightarrow{Z} \emptyset$	
8	R6	Ca independent IP3 degradation	$A \longrightarrow \emptyset$	
9	R7	Phosphorylase kinase activity	$\emptyset \xrightarrow{Z} GP$	
10	R8	Phosphatase activity	$GP \longrightarrow \emptyset$	

6.1 Reaction vin

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

Name Calcium Influx

Reaction equation

$$\mathrm{EC} \longrightarrow \mathrm{Z} \tag{1}$$

Reactant

Table 6: Properties of each reactant.

Id	Name	SBO
EC	Extracellular Calcium	

Product

Table 7: Properties of each product.

Id	Name	SBO
Z	Cytosolic Calcium	

Kinetic Law

Derived unit $\mu\mathrm{mol} \cdot (3600\ \mathrm{s})^{-1}$

$$v_1 = \mathrm{vol}\,(\mathrm{extracellular}) \cdot (\mathrm{v0} + \mathrm{v1} \cdot \mathrm{beta}) \tag{2}$$

6.2 Reaction R2

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

Name Calcium transport to internal store

Reaction equation

$$\mathrm{Z} \longrightarrow \mathrm{Y} \tag{3}$$

Reactant

Table 8: Properties of each reactant.

Id	Name	SBO
Z	Cytosolic Calcium	

Product

Table 9: Properties of each product.

Id	Name	SBO
Y	Intravesicular Calcium	

Kinetic Law

Derived unit $1.0000000000000024 \cdot 10^{-6}\ \mathrm{mol} \cdot (3600\ \mathrm{s})^{-1}$

$$v_2 = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \frac{\mathrm{Vm2} \cdot [\mathrm{Z}]^2}{\mathrm{K2}^2 + [\mathrm{Z}]^2} \tag{4}$$

6.3 Reaction R3

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

Name Calcium transport to cytosol

Reaction equation

$$\mathrm{Y} \xrightarrow{\mathrm{A}} \mathrm{Z} \tag{5}$$

Reactant

Table 10: Properties of each reactant.

Id	Name	SBO
Y	Intravesicular Calcium	

Modifier

Table 11: Properties of each modifier.

Id	Name	SBO
A	IP3	

Product

Table 12: Properties of each product.

Id	Name	SBO
Z	Cytosolic Calcium	

Kinetic Law

Derived unit $1.0000000000000027 \cdot 10^{-6}\ \mathrm{mol} \cdot (3600\ \mathrm{s})^{-1}$

$$v_3 = \frac{\mathrm{vol\,(intravesicular)} \cdot \mathrm{Vm3} \cdot [\mathrm{A}]^4 \cdot [\mathrm{Y}]^2 \cdot [\mathrm{Z}]^{\mathrm{m}}}{\left(\mathrm{Ka}^4 + [\mathrm{A}]^4\right) \cdot \left(\mathrm{Ky}^2 + [\mathrm{Y}]^2\right) \cdot \left(\mathrm{Kz}^{\mathrm{m}} + [\mathrm{Z}]^{\mathrm{m}}\right)} \tag{6}$$

6.4 Reaction Rkf

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

Name Calcium leak

Reaction equation

$$\mathrm{Y} \longrightarrow \mathrm{Z} \tag{7}$$

Reactant

Table 13: Properties of each reactant.

Id	Name	SBO
Y	Intravesicular Calcium	

Product

Table 14: Properties of each product.

Id	Name	SBO
Z	Cytosolic Calcium	

Kinetic Law

Derived unit $(3600\ \mathrm{s})^{-1} \cdot \mu\mathrm{mol}$

$$v_4 = \mathrm{vol}\,(\mathrm{intravesicular}) \cdot \mathrm{Kf} \cdot [\mathrm{Y}] \tag{8}$$

6.5 Reaction Rkz

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

Name Calcium efflux

Reaction equation

$$\mathrm{Z} \longrightarrow \mathrm{EC} \tag{9}$$

Reactant

Table 15: Properties of each reactant.

Id	Name	SBO
Z	Cytosolic Calcium	

Product

Table 16: Properties of each product.

Id	Name	SBO
EC	Extracellular Calcium	

Kinetic Law

Derived unit $(3600\ \mathrm{s})^{-1} \cdot \mu\mathrm{mol}$

$$v_5 = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{K} \cdot [\mathrm{Z}] \tag{10}$$

6.6 Reaction R4

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

Name Agonist stimulated production of IP3

Reaction equation

$$\emptyset \longrightarrow \mathrm{A} \tag{11}$$

Product

Table 17: Properties of each product.

Id	Name	SBO
A	IP3	

Kinetic Law

Derived unit $\mu\mathrm{mol} \cdot (3600\ \mathrm{s})^{-1}$

$$v_6 = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{beta} \cdot \mathrm{V4} \tag{12}$$

6.7 Reaction R5

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

Name Ca-dependant IP3 degradation

Reaction equation

$$\mathrm{A} \xrightarrow{\mathrm{Z}} \emptyset \tag{13}$$

Reactant

Table 18: Properties of each reactant.

Id	Name	SBO
A	IP3	

Modifier

Table 19: Properties of each modifier.

Id	Name	SBO
Z	Cytosolic Calcium	

Kinetic Law

Derived unit $1.0000000000000022 \cdot 10^{-6}\ \mathrm{mol} \cdot (3600\ \mathrm{s})^{-1}$

$$v_7 = \frac{\mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{Vm5} \cdot [\mathrm{A}]^{\mathrm{p}} \cdot [\mathrm{Z}]^{\mathrm{n}}}{(\mathrm{K5}^{\mathrm{p}} + [\mathrm{A}]^{\mathrm{p}}) \cdot (\mathrm{Kd}^{\mathrm{n}} + [\mathrm{Z}]^{\mathrm{n}})} \tag{14}$$

6.8 Reaction R6

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

Name Ca independent IP3 degradation

Reaction equation

$$\mathrm{A} \longrightarrow \emptyset \tag{15}$$

Reactant

Table 20: Properties of each reactant.

Id	Name	SBO
A	IP3	

Kinetic Law

Derived unit $(3600\ \mathrm{s})^{-1} \cdot \mu\mathrm{mol}$

$$v_8 = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{epsilon} \cdot [\mathrm{A}] \tag{16}$$

6.9 Reaction R7

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

Name Phosphorylase kinase activity

Reaction equation

$$\emptyset \xrightarrow{\mathrm{Z}} \mathrm{GP} \tag{17}$$

Modifier

Table 21: Properties of each modifier.

Id	Name	SBO
Z	Cytosolic Calcium	

Product

Table 22: Properties of each product.

Id	Name	SBO
GP	Glycogen Phosphorylase	

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \frac{\mathrm{Vpm1} \cdot \left(1 + \frac{\mathrm{gamma} \cdot [\mathrm{Z}]^4}{\mathrm{Ka5}^4 + [\mathrm{Z}]^4}\right) \cdot (1 - [\mathrm{GP}])}{\frac{\mathrm{K1}}{1 + \frac{[\mathrm{Z}]^4}{\mathrm{Ka6}^4}} + 1 - [\mathrm{GP}]} \tag{18}$$

6.10 Reaction R8

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

Name Phosphatase activity

Reaction equation

$$\mathrm{GP} \longrightarrow \emptyset \tag{19}$$

Reactant

Table 23: Properties of each reactant.

Id	Name	SBO
GP	Glycogen Phosphorylase	

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \frac{\mathrm{Vpm2} \cdot \left(1 + \frac{\mathrm{alpha{\cdot}G}}{\mathrm{Ka1{+}G}}\right) \cdot [\mathrm{GP}]}{\frac{\mathrm{Kp2}}{1+\frac{\mathrm{G}}{\mathrm{Ka2}}} + [\mathrm{GP}]} \tag{20}$$

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.

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.

7.1 Species EC

Name Extracellular Calcium

Initial concentration $1000\ \mu\mathrm{mol} \cdot \mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in vin and as a product in Rkz), which do not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{EC} = 0 \tag{21}$$

7.2 Species Z

Name Cytosolic Calcium

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

This species takes part in seven reactions (as a reactant in R2, Rkz and as a product in vin, R3, Rkf and as a modifier in R5, R7).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Z} = v_1 + v_3 + v_4 - v_2 - v_5 \tag{22}$$

7.3 Species A

Name IP3

Initial concentration $0.45\ \mu\mathrm{mol} \cdot \mathrm{l}^{-1}$

This species takes part in four reactions (as a reactant in R5, R6 and as a product in R4 and as a modifier in R3).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{A} = v_6 - v_7 - v_8 \tag{23}$$

7.4 Species Y

Name Intravesicular Calcium

Initial concentration $0.36\ \mu\text{mol}\cdot\text{l}^{-1}$

This species takes part in three reactions (as a reactant in R3, Rkf and as a product in R2).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Y} = v_2 - v_3 - v_4 \tag{24}$$

7.5 Species GP

Name Glycogen Phosphorylase

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

This species takes part in two reactions (as a reactant in R8 and as a product in R7).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{GP} = v_9 - v_{10} \tag{25}$$

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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