SBML Model Report

Model name: "Dupont1992_Ca_dpt_protein_phospho"

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1 General Overview

This is a document in SBML Level 2 Version 1 format. This model was created by Harish Dharuri[1] at April 19th 2007 at 10:14 a. m. and last time modified at April sixth 2014 at ten o' clock in the afternoon. 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	4
events	0	constraints	0
reactions	7	function definitions	0
global parameters	19	unit definitions	2
rules	1	initial assignments	0

Model Notes

Model reproduces Fig 4 of the paper. For fraction of phosphorylated protein, W_star, the model reproduces panel b in the same figure. Model successfully tested on MathSBML and Jarnac.

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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 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 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
`cytosol`	cytosol		3	1	litre	☑	
`store`	store		3	1	litre	☑	`cytosol`

3.1 Compartment `cytosol`

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

Name cytosol

3.2 Compartment `store`

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

Name store

4 Species

This model contains four 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
`Z`		`cytosol`	$\mu mol \cdot l^{-1}$	⊟	⊟
`Y`		`store`	$\mu mol \cdot l^{-1}$	⊟	⊟
`Wt`	Total Protein	`cytosol`	$\mu mol \cdot l^{-1}$	⊟	⊟
`W_star`	Phosphorylated protein	`cytosol`	$\mu mol \cdot l^{-1}$	⊟	⊟

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5 Parameters

This model contains 19 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
v0			1.00		☑
Vm2			65.00		☑
n			2.00		☑
Kp			1.00		☑
Vm3			500.00		☑
m			2.00		☑
Kr			2.00		☑
K_A			0.90		☑
kf			1.00		☑
k			10.00		☑
p			4.00		☑
vk			0.00		☐
vMK			20.00		☐
vp			2.50		☑
Ka			2.50		☑
q			1.00		☑
K1			0.01		☑
K2			0.01		☑
v1_beta			2.70		☑

6 Rule

This is an overview of one rule.

6.1 Rule vk

Rule vk is an assignment rule for parameter vk:

$$\mathrm{vk} = \frac{\mathrm{vMK} \cdot [\mathrm{Z}]^{\mathrm{q}}}{\mathrm{Ka}^{\mathrm{q}} + [\mathrm{Z}]^{\mathrm{q}}} \tag{1}$$

7 Reactions

This model contains seven 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	R0	Calcium influx	$\emptyset \longrightarrow Z$	
2	R1	InsP3 dependent Ca influx	$\emptyset \longrightarrow Z$	
3	R2	ATP driven pumping of Ca into store	$Z \longrightarrow Y$	
4	R3	ATP driven pumping into cytosol	$Y \longrightarrow Z$	
5	Rf	Calcium leak	$Y \longrightarrow Z$	
6	R_eff	Ca efflux	$Z \longrightarrow \emptyset$	
7	Protein_Phosphorylation	Protein Phosphorylation	$\emptyset \underset{}{\overset{Wt}{\rightleftharpoons}} W\_star$	

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7.1 Reaction R0

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

Name Calcium influx

Reaction equation

$$\emptyset \longrightarrow \mathrm{Z} \tag{2}$$

Product

Table 6: Properties of each product.

Id	Name	SBO
Z		

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{v0} \tag{3}$$

7.2 Reaction R1

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

Name InsP3 dependent Ca influx

Reaction equation

$$\emptyset \longrightarrow \mathrm{Z} \tag{4}$$

Product

Table 7: Properties of each product.

Id	Name	SBO
Z		

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{v1\_beta} \tag{5}$$

7.3 Reaction R2

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

Name ATP driven pumping of Ca into store

Reaction equation

$$\mathrm{Z} \longrightarrow \mathrm{Y} \tag{6}$$

Reactant

Table 8: Properties of each reactant.

Id	Name	SBO
Z		

Product

Table 9: Properties of each product.

Id	Name	SBO
Y		

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \frac{\mathrm{Vm2} \cdot [\mathrm{Z}]^{\mathrm{n}}}{\mathrm{Kp}^{\mathrm{n}} + [\mathrm{Z}]^{\mathrm{n}}} \tag{7}$$

7.4 Reaction R3

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

Name ATP driven pumping into cytosol

Reaction equation

$$\mathrm{Y} \longrightarrow \mathrm{Z} \tag{8}$$

Reactant

Table 10: Properties of each reactant.

Id	Name	SBO
Y		

Product

Table 11: Properties of each product.

Id	Name	SBO
Z		

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \mathrm{vol}(\mathrm{store}) \cdot \frac{\mathrm{Vm3} \cdot [\mathrm{Y}]^{\mathrm{m}} \cdot [\mathrm{Z}]^{\mathrm{p}}}{(\mathrm{Kr}^{\mathrm{m}} + [\mathrm{Y}]^{\mathrm{m}}) \cdot (\mathrm{K\_A}^{\mathrm{p}} + [\mathrm{Z}]^{\mathrm{p}})} \tag{9}$$

7.5 Reaction Rf

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

Name Calcium leak

Reaction equation

$$\mathrm{Y} \longrightarrow \mathrm{Z} \tag{10}$$

Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
Y		

Product

Table 13: Properties of each product.

Id	Name	SBO
Z		

Id	Name	SBO

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \mathrm{vol}\,(\mathrm{store}) \cdot \mathrm{kf} \cdot [\mathrm{Y}] \tag{11}$$

7.6 Reaction R_eff

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

Name Ca efflux

Reaction equation

$$\mathrm{Z} \longrightarrow \emptyset \tag{12}$$

Reactant

Table 14: Properties of each reactant.

Id	Name	SBO
Z		

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{k} \cdot [\mathrm{Z}] \tag{13}$$

7.7 Reaction Protein_Phosphorylation

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

Name Protein Phosphorylation

Reaction equation

$$\emptyset \underset{}{\overset{\mathrm{Wt}}{\rightleftharpoons}} \mathrm{W\_star} \tag{14}$$

Modifier

Table 15: Properties of each modifier.

Id	Name	SBO
Wt	Total Protein	

Product

Table 16: Properties of each product.

Id	Name	SBO
W_star	Phosphorylated protein	

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \frac{\mathrm{vp}}{[\mathrm{Wt}]} \cdot \left(\frac{\mathrm{vk}}{\mathrm{vp}} \cdot \frac{1 - [\mathrm{W\_star}]}{\mathrm{K1} + 1 - [\mathrm{W\_star}]} - \frac{[\mathrm{W\_star}]}{\mathrm{K2} + [\mathrm{W\_star}]} \right) \tag{15}$$

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 Z

Initial concentration $0.15\ \mu\mathrm{mol} \cdot \mathrm{l}^{-1}$

This species takes part in six reactions (as a reactant in R2, R_eff and as a product in R0, R1, R3, Rf).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Z} = v_1 + v_2 + v_4 + v_5 - v_3 - v_6 \tag{16}$$

8.2 Species Y

Initial concentration $1.6\ \mu\text{mol}\cdot\text{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Y} = v_3 - v_4 - v_5 \tag{17}$$

8.3 Species Wt

Name Total Protein

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

This species takes part in one reaction (as a modifier in Protein_Phosphorylation).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Wt} = 0 \tag{18}$$

8.4 Species W_star

Name Phosphorylated protein

This species takes part in one reaction (as a product in Protein_Phosphorylation).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{W\_star} = v_7 \tag{19}$$

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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