## **SBML Model Report**

# Model name: "Dupont1991\_CaOscillation"



May 6, 2016

#### 1 General Overview

This is a document in SBML Level 2 Version 1 format. This model was created by Enuo He<sup>1</sup> at May 22<sup>nd</sup> 2007 at 1:36 p. m. and last time modified at July fifth 2012 at 4:48 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	2
events	1	constraints	0
reactions	6	function definitions	0
global parameters	15	unit definitions	1
rules	1	initial assignments	0

#### **Model Notes**

This model is according to the paper *Signal-induced Ca2+ oscillations: Properties of a model based on Ca2+-induced Ca2+ release.* Figure 4B in the paper has been reproduced by Road-Runner and MathSBML. Damped Ca2+ oscillations elicited by a transient pulse of InsP3 applied intracellularly to a resting, non-oscillatory cell.

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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 four are predefined by SBML and not mentioned in the model.

#### 2.1 Unit substance

Name microM

**Definition** µmol

#### 2.2 Unit volume

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

Definition 1

#### 2.3 Unit area

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

**Definition** m<sup>2</sup>

### 2.4 Unit length

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

**Definition** m

#### 2.5 Unit time

**Notes** Second is the predefined SBML unit for time.

**Definition** s

# 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	$\overline{\mathbf{Z}}$	
$\verb intracellular_Ca_storepool \\$			3	1	litre		

## 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.

## 3.3 Compartment intracellular\_Ca\_storepool

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

# 4 Species

This model contains two 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 Condi- tion
z y	Ca in the cytosol Ca in the InsP3-insensitive pool	Cytosol intracellular_Ca- _storepool	$\begin{array}{l} \mu mol \cdot l^{-1} \\ \mu mol \cdot l^{-1} \end{array}$		

#### **5 Parameters**

This model contains 15 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
v0			1.0		
v1			7.3		$ \mathbf{Z} $
VM2			65.0		$\mathbf{Z}$
VM3			500.0		$\mathbf{Z}$
KR			2.0		$\mathbf{Z}$
KA			0.9		
K2			1.0		$\mathbf{Z}$
kf			1.0		$ \mathbf{Z} $
k			10.0		$ \mathbf{Z} $
n			2.0		$ \mathbf{Z} $
m			2.0		$ \mathbf{Z} $
p			4.0		$\square$
tstim	stimulation time		4.0		$\overline{\mathbf{Z}}$
beta			0.0		
flag			0.0		

### 6 Rule

This is an overview of one rule.

#### 6.1 Rule beta

Rule beta is an assignment rule for parameter beta:

$$beta = flag \cdot 0.96 \cdot exp(-0.2 \cdot (time - tstim))$$
 (1)

**Notes** According to the legend of Figure 4B, beta decays from the initial value beta\_f=96% according to the equation beta=beta\_f\*exp[-0.2\*(t-tp)]. and tp=4s.

## 7 Event

This is an overview of one event. 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

Trigger condition  $time > tstim \tag{2} \label{2}$  Assignment

flag = 1

(3)

# 8 Reactions

This model contains six 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

N₀	Id	Name	Reaction Equation	SBO
1	reaction- _0000001	InsP3 modulated release of Ca from the InsP3 sensitive store	$\emptyset \longrightarrow z$	
2	reaction- _0000002	Constant input of Ca from the extracellular medium	$\emptyset \longrightarrow z$	
3	reaction- _0000003	Leak Ca from pool to cytosol	$y \longrightarrow z$	
4	reaction- _0000004	Pumping Ca into the InsP3-insensitive store	$z \longrightarrow y$	
5	reaction- _0000005	Release of Ca from the pool into the cytosol	$y \longrightarrow z$	
6	reaction- _0000006	Transport of cytosolic ca into the extracellular medium	$z \longrightarrow \emptyset$	

#### 8.1 Reaction reaction\_0000001

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

Name InsP3 modulated release of Ca from the InsP3 sensitive store

### **Reaction equation**

$$\emptyset \longrightarrow z$$
 (4)

#### **Product**

Table 6: Properties of each product.

	*	
Id	Name	SBO
z	Ca in the cytosol	

#### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_1 = v1 \cdot beta \cdot vol (Cytosol)$$
 (5)

#### **8.2 Reaction** reaction\_0000002

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

Name Constant input of Ca from the extracellular medium

#### **Reaction equation**

$$\emptyset \longrightarrow z$$
 (6)

#### **Product**

Table 7: Properties of each product.

Id	Name	SBO
z	Ca in the cytosol	

#### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_2 = v0 \cdot vol(Cytosol) \tag{7}$$

#### 8.3 Reaction reaction\_0000003

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

Name Leak Ca from pool to cytosol

### **Reaction equation**

$$y \longrightarrow z$$
 (8)

#### Reactant

Table 8: Properties of each reactant.

Id	Name	SBO
У	Ca in the InsP3-insensitive pool	

#### **Product**

Table 9: Properties of each product.

Id	Name	SBO
z	Ca in the cytosol	

#### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_3 = kf \cdot [y] \cdot vol(Cytosol) \tag{9}$$

## 8.4 Reaction reaction\_0000004

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

Name Pumping Ca into the InsP3-insensitive store

### **Reaction equation**

$$z \longrightarrow y$$
 (10)

#### Reactant

Table 10: Properties of each reactant.

Id	Name	SBO
z	Ca in the cytosol	

#### **Product**

Table 11: Properties of each product.

	1 1	
Id	Name	SBO
У	Ca in the InsP3-insensitive pool	

#### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_4 = \frac{\text{vol}\left(\text{intracellular\_Ca\_storepool}\right) \cdot \text{VM2} \cdot [z]^n}{\text{K2}^n + [z]^n} \tag{11}$$

### 8.5 Reaction reaction\_0000005

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

Name Release of Ca from the pool into the cytosol

### **Reaction equation**

$$y \longrightarrow z$$
 (12)

#### Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
У	Ca in the InsP3-insensitive pool	

#### **Product**

Table 13: Properties of each product.

Id	Name	SBO
z	Ca in the cytosol	

Id	Name	SBO

#### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_5 = \text{vol}\left(\text{Cytosol}\right) \cdot \text{VM3} \cdot \frac{[y]^m}{KR^m + [y]^m} \cdot \frac{[z]^p}{KA^p + [z]^p}$$
(13)

#### 8.6 Reaction reaction\_0000006

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

Name Transport of cytosolic ca into the extracellular medium

#### **Reaction equation**

$$z \longrightarrow \emptyset$$
 (14)

#### Reactant

Table 14: Properties of each reactant.

Id	Name	SBO
z	Ca in the cytosol	

#### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_6 = \mathbf{k} \cdot [\mathbf{z}] \cdot \text{vol} (\text{extracellular})$$
 (15)

# 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 z

Name Ca in the cytosol

Initial concentration  $0.1 \, \mu mol \cdot l^{-1}$ 

This species takes part in six reactions (as a reactant in reaction\_0000004, reaction\_0000006 and as a product in reaction\_0000001, reaction\_0000002, reaction\_0000003, reaction\_0000005).

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

#### 9.2 Species y

Name Ca in the InsP3-insensitive pool

Initial concentration  $1.4 \, \mu mol \cdot l^{-1}$ 

This species takes part in three reactions (as a reactant in reaction\_0000003, reaction\_0000005 and as a product in reaction\_0000004).

$$\frac{d}{dt}y = |v_4| - |v_3| - |v_5| \tag{17}$$

 $\mathfrak{BML2}^{d}$  was developed by Andreas Dräger<sup>a</sup>, Hannes Planatscher<sup>a</sup>, Dieudonné M Wouamba<sup>a</sup>, Adrian Schröder<sup>a</sup>, Michael Hucka<sup>b</sup>, Lukas Endler<sup>c</sup>, Martin Golebiewski<sup>d</sup> and Andreas Zell<sup>a</sup>. Please see http://www.ra.cs.uni-tuebingen.de/software/SBML2LaTeX for more information.

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