

# SBML Model Report

Model identifier: “NTyamada\_v1\_36”



July 2, 2015

## 1 General Overview

This is a document in SBML Level 2 Version 4 format. Table 1 shows an overview of the quantities of all components of this model.

Table 1: The SBML components in this model.  
All components are described in more detail in the following sections.

Element	Quantity	Element	Quantity
compartment types	0	compartments	1
species types	0	species	9
events	5	constraints	0
reactions	5	function definitions	0
global parameters	25	unit definitions	8
rules	4	initial assignments	0

## Model Notes

## 2 Unit Definitions

This is an overview of eight unit definitions.

### 2.1 Unit per\_mM\_per\_ms

**Name** per\_mM\_per\_ms

**Definition** mmol·l<sup>-1</sup>·ms<sup>-1</sup>

## 2.2 Unit per\_ms

**Name** per\_ms

**Definition**  $\text{ms}^{-1}$

## 2.3 Unit substance

**Name** substance

**Definition** mol

## 2.4 Unit volume

**Name** volume

**Definition** l

## 2.5 Unit area

**Name** area

**Definition**  $\text{m}^2$

## 2.6 Unit length

**Name** length

**Definition** m

## 2.7 Unit time

**Name** time

**Definition** s

## 2.8 Unit ms

**Name** ms

**Definition** ms

## 3 Compartment

This model contains one compartment.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
default			3	1	litre	<input checked="" type="checkbox"/>	

### 3.1 **Compartment** default

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

## 4 Species

This model contains nine species. The boundary condition of two of these species is set to true so that these species' amount cannot be changed by any reaction. 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
XX	XX	default	$\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
Ca	Ca	default	mol	<input type="checkbox"/>	<input checked="" type="checkbox"/>
XXC	XXC	default	mol	<input type="checkbox"/>	<input type="checkbox"/>
XX2C	XX2C	default	mol	<input type="checkbox"/>	<input type="checkbox"/>
XX3C	XX3C	default	mol	<input type="checkbox"/>	<input type="checkbox"/>
XX4C	XX4C	default	mol	<input type="checkbox"/>	<input type="checkbox"/>
YY	YY	default	$\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
YYC	YYC	default	mol	<input type="checkbox"/>	<input type="checkbox"/>
nAchR_Current	nAchR_Current	default	mol	<input type="checkbox"/>	<input checked="" type="checkbox"/>

## 5 Parameters

This model contains 25 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
konX	konX		500.000	$\text{mmol} \cdot \text{l}^{-1} \cdot \text{ms}^{-1}$	<input checked="" type="checkbox"/>
koffX	koffX		100.000	$\text{ms}^{-1}$	<input checked="" type="checkbox"/>
konY	konY		10.000	$\text{mmol} \cdot \text{l}^{-1} \cdot \text{ms}^{-1}$	<input checked="" type="checkbox"/>
koffY	koffY		0.150	$\text{ms}^{-1}$	<input checked="" type="checkbox"/>
kk2	kk2		1.000	$\text{mmol} \cdot \text{l}^{-1} \cdot \text{ms}^{-1}$	<input checked="" type="checkbox"/>
kk3	kk3		10.000	$\text{ms}^{-1}$	<input checked="" type="checkbox"/>
CONSERVATION	CONSERVATION		0.000	dimensionless	<input type="checkbox"/>
CONSERVATION2	CONSERVATION2		0.000	dimensionless	<input type="checkbox"/>
totalNbOfVesicles	totalNbOfVesicles		270.000	dimensionless	<input type="checkbox"/>
vesicleReleased	vesicleReleased		0.000	dimensionless	<input type="checkbox"/>
totNbOfNTperVesicle	totNbOfNTperVesicle		3000.000	dimensionless	<input checked="" type="checkbox"/>
vesicleCount	vesicleCount		0.000	dimensionless	<input type="checkbox"/>
NT	NT		0.000	dimensionless	<input type="checkbox"/>
timeOfLastRelease	timeOfLastRelease		0.000	ms	<input type="checkbox"/>
ReleaseRate	ReleaseRate		0.000	$\text{mmol} \cdot \text{l}^{-1} \cdot \text{ms}^{-1}$	<input type="checkbox"/>
refractoryPeriod	refractoryPeriodDuration		5.000	ms	<input checked="" type="checkbox"/>
refractoryTime	refractoryTime		0.000	dimensionless	<input type="checkbox"/>
probabilisticRelease	probabilisticRelease		0.000	dimensionless	<input checked="" type="checkbox"/>
numberOfSimulations	numberOfSimulations		1.000	dimensionless	<input checked="" type="checkbox"/>
seed	seed		1.000	dimensionless	<input checked="" type="checkbox"/>
initialReleaseProba	initialReleaseProba		0.300	dimensionless	<input checked="" type="checkbox"/>
threshold- _nAchRCurrent	threshold- _nAchRCurrent		$5 \cdot 10^{-6}$	dimensionless	<input checked="" type="checkbox"/>
test	test		0.000	$\text{mmol} \cdot \text{l}^{-1} \cdot \text{ms}^{-1}$	<input type="checkbox"/>
increaseProba	increaseProba		0.400	dimensionless	<input checked="" type="checkbox"/>
releaseProba	releaseProba		0.000	dimensionless	<input type="checkbox"/>

## 6 Rules

This is an overview of four rules.

### 6.1 Rule 1

Rule is an assignment rule for parameter CONSERVATION:

$$\text{CONSERVATION} = 1 - [\text{XXC}] - [\text{XX2C}] - [\text{XX3C}] - [\text{XX4C}] \quad (1)$$

## 6.2 Rule 2

Rule is an assignment rule for parameter CONSERVATION2:

$$\text{CONSERVATION2} = 1 - \text{YYC} \quad (2)$$

## 6.3 Rule 3

Rule is a rate rule for parameter vesicleReleased:

$$\frac{d}{dt} \text{vesicleReleased} = \text{ReleaseRate} \cdot \text{totalNbOfVesicles} \quad (3)$$

**Derived unit**  $\text{l}^{-1} \cdot \text{mmol} \cdot \text{ms}^{-1}$

## 6.4 Rule 4

Rule is a rate rule for parameter ReleaseRate:

$$\frac{d}{dt} \text{ReleaseRate} = \text{kk2} \cdot [\text{XX4C}] \cdot \text{YYC} - \text{kk3} \cdot \text{ReleaseRate} \quad (4)$$

# 7 Events

This is an overview of five 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 `release_ON`

**Name** `release_ON`

**Trigger** The following condition decides whether this trigger may fire:

$$(\text{vesicleReleased} > 0.98) \wedge (\text{refractoryTime} = 0) \quad (5)$$

**Delay**

$$0 \quad (6)$$

**Time unit of the delay** `invalid`

**Assignments** The values of the assignment formulas are computed at the moment this event fires, not after the delay.

$$\text{vesicleCount} = \text{vesicleCount} + 1 \quad (7)$$

$$\text{vesicleReleased} = 0 \quad (8)$$

$$\text{NT} = \text{totNbOfNTperVesicle} \quad (9)$$

$$\text{timeOfLastRelease} = \text{time} \quad (10)$$

$$\text{refractoryTime} = 1 \quad (11)$$

## 7.2 Event `release_OFF`

**Name** `release_OFF`

**Trigger** The following condition decides whether this trigger may fire:

$$\text{time} - \text{timeOfLastRelease} \geq 5 \cdot 10^{-4} \quad (12)$$

**Delay**

$$0 \quad (13)$$

**Time unit of the delay** `invalid`

**Assignment** The values of the assignment formula is computed at the moment this event fires, not after the delay.

$$\text{NT} = 0 \quad (14)$$

## 7.3 Event `refractory_period_END`

**Name** `refractory_period_END`

**Trigger** The following condition decides whether this trigger may fire:

$$\begin{aligned} &(\text{time} - \text{timeOfLastRelease} \geq \text{refractoryPeriodDuration}) \\ &\wedge (\text{timeOfLastRelease} \neq 0) \end{aligned} \quad (15)$$

**Delay**

$$0 \quad (16)$$

**Time unit of the delay** `invalid`

**Assignments** The values of the assignment formulas are computed at the moment this event fires, not after the delay.

$$\text{refractoryTime} = 0 \quad (17)$$

$$\text{vesicleReleased} = 0 \quad (18)$$

## 7.4 Event `proba_UP`

**Name** `proba_UP`

**Trigger** The following condition decides whether this trigger may fire:

$$|\text{nAchR\_Current}| > |\text{threshold\_nAchRCurrent}| \quad (19)$$

**Delay** 0 (20)

**Time unit of the delay** invalid

**Assignments** The values of the assignment formulas are computed at the moment this event fires, not after the delay.

$$\text{releaseProba} = \text{initialReleaseProba} + \text{increaseProba} \quad (21)$$

$$\text{test} = \text{nAchR\_Current} \quad (22)$$

### 7.5 Event `proba_DOWN`

**Name** `proba_DOWN`

**Trigger** The following condition decides whether this trigger may fire:

$$|\text{nAchR\_Current}| \leq |\text{threshold\_nAchRCurrent}| \quad (23)$$

**Delay** 0 (24)

**Time unit of the delay** invalid

**Assignment** The values of the assignment formula is computed at the moment this event fires, not after the delay.

$$\text{releaseProba} = \text{initialReleaseProba} \quad (25)$$



## 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 one or more modifiers, the identifiers of the modifier species are written above the reaction arrow.

Table 5: Overview of all reactions

Nº	Id	Name	Reaction Equation	SBO
1	fast1		$XX + Ca \rightleftharpoons XXC$	
2	fast2		$XXC + Ca \rightleftharpoons XX2C$	
3	fast3		$XX2C + Ca \rightleftharpoons XX3C$	
4	fast4		$XX3C + Ca \rightleftharpoons XX4C$	
5	slow1		$YY + Ca \rightleftharpoons YYC$	

## 8.1 Reaction *fast1*

This is a reversible reaction of two reactants forming one product.

### Reaction equation



### Reactants

Table 6: Properties of each reactant.

Id	Name	SBO
XX	XX	
Ca	Ca	

### Product

Table 7: Properties of each product.

Id	Name	SBO
XXC	XXC	

### Kinetic Law

**Derived unit** contains undeclared units

$$v_1 = 4 \cdot \text{konX} \cdot \text{CONSERVATION} \cdot \text{Ca} - 1 \cdot \text{koffX} \cdot [\text{XXC}] \quad (27)$$

## 8.2 Reaction *fast2*

This is a reversible reaction of two reactants forming one product.

### Reaction equation



### Reactants

Table 8: Properties of each reactant.

Id	Name	SBO
XXC	XXC	
Ca	Ca	

## Product

Table 9: Properties of each product.

Id	Name	SBO
XX2C	XX2C	

## Kinetic Law

**Derived unit** contains undeclared units

$$v_2 = 3 \cdot \text{konX} \cdot [\text{XXC}] \cdot \text{Ca} - 2 \cdot \text{koffX} \cdot [\text{XX2C}] \quad (29)$$

## 8.3 Reaction `fast3`

This is a reversible reaction of two reactants forming one product.

### Reaction equation



## Reactants

Table 10: Properties of each reactant.

Id	Name	SBO
XX2C	XX2C	
Ca	Ca	

## Product

Table 11: Properties of each product.

Id	Name	SBO
XX3C	XX3C	

### Kinetic Law

**Derived unit** contains undeclared units

$$v_3 = 2 \cdot \text{konX} \cdot [\text{XX2C}] \cdot \text{Ca} - 3 \cdot \text{koffX} \cdot [\text{XX3C}] \quad (31)$$

### 8.4 Reaction fast4

This is a reversible reaction of two reactants forming one product.

### Reaction equation



### Reactants

Table 12: Properties of each reactant.

Id	Name	SBO
XX3C	XX3C	
Ca	Ca	

### Product

Table 13: Properties of each product.

Id	Name	SBO
XX4C	XX4C	

### Kinetic Law

**Derived unit** contains undeclared units

$$v_4 = 1 \cdot \text{konX} \cdot [\text{XX3C}] \cdot \text{Ca} - 4 \cdot \text{koffX} \cdot [\text{XX4C}] \quad (33)$$

## 8.5 Reaction `slow1`

This is a reversible reaction of two reactants forming one product.

### Reaction equation



### Reactants

Table 14: Properties of each reactant.

Id	Name	SBO
YY	YY	
Ca	Ca	

### Product

Table 15: Properties of each product.

Id	Name	SBO
YYC	YYC	

### Kinetic Law

**Derived unit** contains undeclared units

$$v_5 = k_{onY} \cdot CONSERVATION2 \cdot Ca - k_{offY} \cdot YYC \quad (35)$$

## 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 a 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 XX

**Name** XX

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

**Charge** 0

This species takes part in one reaction (as a reactant in [fast1](#)).

$$\frac{d}{dt}XX = -v_1 \quad (36)$$

### 9.2 Species Ca

**Name** Ca

**Initial amount**  $5 \cdot 10^{-5} \text{ mol}$

**Charge** 0

This species takes part in five reactions (as a reactant in [fast1](#), [fast2](#), [fast3](#), [fast4](#), [slow1](#)), which do not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{d}{dt}Ca = 0 \quad (37)$$

### 9.3 Species XXC

**Name** XXC

**Initial amount** 0 mol

**Charge** 0

This species takes part in two reactions (as a reactant in [fast2](#) and as a product in [fast1](#)).

$$\frac{d}{dt}XXC = v_1 - v_2 \quad (38)$$

### 9.4 Species XX2C

**Name** XX2C

**Initial amount** 0 mol

**Charge** 0

This species takes part in two reactions (as a reactant in [fast3](#) and as a product in [fast2](#)).

$$\frac{d}{dt}XX2C = v_2 - v_3 \quad (39)$$

### 9.5 Species XX3C

**Name** XX3C

**Initial amount** 0 mol

**Charge** 0

This species takes part in two reactions (as a reactant in `fast4` and as a product in `fast3`).

$$\frac{d}{dt}XX3C = v_3 - v_4 \quad (40)$$

### 9.6 Species XX4C

**Name** XX4C

**Initial amount** 0 mol

**Charge** 0

This species takes part in one reaction (as a product in `fast4`).

$$\frac{d}{dt}XX4C = v_4 \quad (41)$$

### 9.7 Species YY

**Name** YY

**Initial concentration** 1 mol · l<sup>-1</sup>

**Charge** 0

This species takes part in one reaction (as a reactant in `slow1`).

$$\frac{d}{dt}YY = -v_5 \quad (42)$$

### 9.8 Species YYC

**Name** YYC

**Initial amount** 0.00332225905256408 mol

**Charge** 0

This species takes part in one reaction (as a product in `slow1`).

$$\frac{d}{dt}YYC = v_5 \quad (43)$$

## 9.9 Species `nAchR_Current`

**Name** `nAchR_Current`

**Initial amount** 0 mol

**Charge** 0

$$\frac{d}{dt}nAchR\_Current = 0 \quad (44)$$

## References

Dräger, A., Planatscher, H., Wouamba, D. M., Schröder, A., Hucka, M., Endler, L., Golebiewski, M., Müller, W., and Zell, A. (2009). SBML2 $\LaTeX$ : Conversion of SBML files into human-readable reports. *Bioinformatics*, **25**(11), 1455–1456. [10.1093/bioinformatics/btp170](https://doi.org/10.1093/bioinformatics/btp170).