SBML Model Report

Model name: "Komarova2005-_TheoreticalFramework_BasicArchitecture"

May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 1 format. This model was created by Enuo He[1] at June fourth 2007 at 3:33 p. m. and last time modified at July fifth 2012 at 4:31 p. m. 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	1
species types	0	species	5
events	1	constraints	0
reactions	7	function definitions	0
global parameters	7	unit definitions	0
rules	0	initial assignments	0

Model Notes

This model according to the paper *A Theoretical Framework for Specificity in Cell Signalling* The model is „basic architecture„ of Figure2A. Figure2B, Figure2C have been reproduced by MathSBML. The reproduced figures are slightly different from the original ones in the paper, the peak of [x2] is higher than 1 and is not decreasing dramatically when [x0]=0. And I think maybe the author shift the or scale the curves.

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2 Unit Definitions

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

2.1 Unit `substance`

Notes Mole is the predefined SBML unit for `substance`.

Definition mol

2.2 Unit `volume`

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

Definition l

2.3 Unit `area`

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

Definition m^2

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 Compartment

This model contains one compartment.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
compartment_0000001	cell		3	1	litre	☑	

3.1 Compartment compartment_0000001

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

Name cell

4 Species

This model contains five 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
x1		compartment_0000001	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
x2		compartment_0000001	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
y2		compartment_0000001	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
x0		compartment_0000001	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
y0		compartment_0000001	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟

5 Parameters

This model contains seven global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
a1			2.0		☑
a2			2.0		☑
b1			1.0		☑
b2			1.0		☑
d1			1.0		☑
d2x			1.0		☑
d2y			1.0		☑

6 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.

6.1 Event `event_0000001`

Notes x0 signaling applied as square pulses of magnitude 1 and duration 1.

Trigger condition

$$\text{time} > 1 \tag{1}$$

Assignment

$$\text{x0} = 0 \tag{2}$$

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	reaction_0000001	x0 activates x1	$\emptyset \xrightarrow{\text{x0}} \text{x1}$	
2	reaction_0000002	y0 activates x1	$\emptyset \xrightarrow{\text{y0}} \text{x1}$	
3	reaction_0000003	x1 activates x2	$\emptyset \xrightarrow{\text{x1}} \text{x2}$	
4	reaction_0000004	x1 activates y2	$\emptyset \xrightarrow{\text{x1}} \text{y2}$	
5	reaction_0000005	x1 deactivation	$\text{x1} \longrightarrow \emptyset$	
6	reaction_0000006	x2 deactivation	$\text{x2} \longrightarrow \emptyset$	
7	reaction_0000007	y2 deactivation	$\text{y2} \longrightarrow \emptyset$	

7.1 Reaction reaction_0000001

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

Name x0 activates x1

Reaction equation

$$\emptyset \xrightarrow{\text{x0}} \text{x1} \tag{3}$$

Modifier

Table 6: Properties of each modifier.

Id	Name	SBO
x0		

Product

Table 7: Properties of each product.

Id	Name	SBO
x1		

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \text{vol}(\text{compartment\_0000001}) \cdot \text{a1} \cdot [\text{x0}] \tag{4}$$

7.2 Reaction reaction_0000002

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

Name y0 activates x1

Reaction equation

$$\emptyset \xrightarrow{\text{y0}} \text{x1} \tag{5}$$

Modifier

Table 8: Properties of each modifier.

Id	Name	SBO
y0		

Product

Table 9: Properties of each product.

Id	Name	SBO
x1		

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \mathrm{vol}\,(\mathrm{compartment\_0000001}) \cdot \mathrm{b1} \cdot [\mathrm{y0}] \tag{6}$$

7.3 Reaction reaction_0000003

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

Name x1 activates x2

Reaction equation

$$\emptyset \xrightarrow{\mathrm{x1}} \mathrm{x2} \tag{7}$$

Modifier

Table 10: Properties of each modifier.

Id	Name	SBO
x1		

Product

Table 11: Properties of each product.

Id	Name	SBO
x2		

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \mathrm{vol}\,(\mathrm{compartment\_0000001}) \cdot [\mathrm{x1}] \cdot \mathrm{a2} \tag{8}$$

7.4 Reaction `reaction_0000004`

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

Name x1 activates y2

Reaction equation

$$\emptyset \xrightarrow{\mathrm{x1}} \mathrm{y2} \tag{9}$$

Modifier

Table 12: Properties of each modifier.

Id	Name	SBO
x1		

Product

Table 13: Properties of each product.

Id	Name	SBO
y2		

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \mathrm{vol}\,(\mathrm{compartment\_0000001}) \cdot [\mathrm{x1}] \cdot \mathrm{b2} \tag{10}$$

7.5 Reaction `reaction_0000005`

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

Name x1 deactivation

Reaction equation

$$\mathrm{x1} \longrightarrow \emptyset \tag{11}$$

Reactant

Table 14: Properties of each reactant.

Id	Name	SBO
x1		

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \mathrm{vol}\,(\mathrm{compartment\_0000001}) \cdot \mathrm{d1} \cdot [\mathrm{x1}] \tag{12}$$

7.6 Reaction reaction_0000006

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

Name x2 deactivation

Reaction equation

$$\mathrm{x2} \longrightarrow \emptyset \tag{13}$$

Reactant

Table 15: Properties of each reactant.

Id	Name	SBO
x2		

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \mathrm{vol}\,(\mathrm{compartment\_0000001}) \cdot \mathrm{d2x} \cdot [\mathrm{x2}] \tag{14}$$

7.7 Reaction reaction_0000007

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

Name y2 deactivation

Reaction equation

$$\mathrm{y2} \longrightarrow \emptyset \tag{15}$$

Reactant

Table 16: Properties of each reactant.

Id	Name	SBO
y2		

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \mathrm{vol}\,(\mathrm{compartment\_0000001}) \cdot \mathrm{d2y} \cdot [\mathrm{y2}] \tag{16}$$

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 `x1`

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

This species takes part in five reactions (as a reactant in `reaction_0000005` and as a product in `reaction_0000001`, `reaction_0000002` and as a modifier in `reaction_0000003`, `reaction_0000004`).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{x1} = v_1 + v_2 - v_5 \tag{17}$$

8.2 Species `x2`

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

This species takes part in two reactions (as a reactant in `reaction_0000006` and as a product in `reaction_0000003`).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{x2} = v_3 - v_6 \tag{18}$$

8.3 Species y2

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

This species takes part in two reactions (as a reactant in reaction_0000007 and as a product in reaction_0000004).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{y2} = v_4 - v_7 \tag{19}$$

8.4 Species x0

Notes x0(t) and y0(t) are the signal functions. The authors assume the network only receives one of the two signals at a time. Thus, if x0(t) is postive for some duration of time, then y0(t) is identically zero, and visa versa.

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

Involved in event event_0000001

This species takes part in one reaction (as a modifier in reaction_0000001).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{x0} = 0 \tag{20}$$

Furthermore, one event influences this species' rate of change.

8.5 Species y0

Notes x0(t) and y0(t) are the signal functions. The authors assume the network only receives one of the two signals at a time. Thus, if y0(t) is postive for some duration of time, then x0(t) is identically zero, and visa versa.

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

This species takes part in one reaction (as a modifier in reaction_0000002).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{y0} = 0 \tag{21}$$

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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