SBML Model Report

Model identifier: "BASE_MODEL_2010_03_08"

July 2, 2015

1 General Overview

This is a document in SBML Level 2 Version 4 format. Table 1 gives 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	6
events	1	constraints	0
reactions	8	function definitions	0
global parameters	21	unit definitions	12
rules	9	initial assignments	0

Model Notes

2 Unit Definitions

This is an overview of twelve unit definitions.

2.1 Unit pS

Name pS

Definition pS

2.2 Unit pA

Name pA

Definition pA

2.3 Unit mV

Name mV

Definition mV

2.4 Unit msec

Name msec

Definition ms

2.5 Unit mM

Name milliMolar

Definition $\mathrm{mmol} \cdot \mathrm{l}^{-1}$

2.6 Unit per_mM_per_msec

Name per_mM_per_msec

Definition $\mathrm{l} \cdot \mathrm{mmol}^{-1} \cdot \mathrm{ms}^{-1}$

2.7 Unit per_msec

Name per_msec

Definition ms^{-1}

2.8 Unit substance

Name substance

Definition mol

2.9 Unit volume

Name volume

Definition l

2.10 Unit `area`

Name area

Definition m^2

2.11 Unit `length`

Name length

Definition m

2.12 Unit `time`

Name 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
`default`			3	1	litre	☑	

3.1 Compartment `default`

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

4 Species

This model contains six 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 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
C1	C1	default	mol	☐	☐
C2	C2	default	mol	☐	☐
C3	C3	default	mol	☐	☐
C4	C4	default	mol	☐	☐
O	O	default	mol	☐	☐
v	v	default	mol	☐	☑

5 Parameters

This model contains 21 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
alpha10	alpha10		4.04	ms^{-1}	☑
alpha20	alpha20		6.70	ms^{-1}	☑
alpha30	alpha30		4.39	ms^{-1}	☑
alpha40	alpha40		17.33	ms^{-1}	☑
beta10	beta10		2.88	ms^{-1}	☑
beta20	beta20		6.30	ms^{-1}	☑
beta30	beta30		8.16	ms^{-1}	☑
beta40	beta40		1.84	ms^{-1}	☑
v1	v1		49.14	mV	☑
v2	v2		42.08	mV	☑
v3	v3		55.31	mV	☑
v4	v4		26.55	mV	☑
alpha1	alpha1		0.00	ms^{-1}	⊟
alpha2	alpha2		0.00	ms^{-1}	⊟
alpha3	alpha3		0.00	ms^{-1}	⊟
alpha4	alpha4		0.00	ms^{-1}	⊟
beta1	beta1		0.00	ms^{-1}	⊟
beta2	beta2		0.00	ms^{-1}	⊟
beta3	beta3		0.00	ms^{-1}	⊟
beta4	beta4		0.00	ms^{-1}	⊟
I	I		0.00	pA	⊟

6 Rules

This is an overview of nine rules.

6.1 Rule 1

Rule is an assignment rule for parameter alpha1:

$$\texttt{alpha1} = \texttt{alpha10} \cdot \exp\left(\frac{\texttt{v}}{\texttt{v1}}\right) \tag{1}$$

6.2 Rule 2

Rule is an assignment rule for parameter `alpha2`:

$$\texttt{alpha2} = \texttt{alpha20} \cdot \exp\left(\frac{\texttt{v}}{\texttt{v2}}\right) \tag{2}$$

6.3 Rule 3

Rule is an assignment rule for parameter `alpha3`:

$$\texttt{alpha3} = \texttt{alpha30} \cdot \exp\left(\frac{\texttt{v}}{\texttt{v3}}\right) \tag{3}$$

6.4 Rule 4

Rule is an assignment rule for parameter `alpha4`:

$$\texttt{alpha4} = \texttt{alpha40} \cdot \exp\left(\frac{\texttt{v}}{\texttt{v4}}\right) \tag{4}$$

6.5 Rule 5

Rule is an assignment rule for parameter `beta1`:

$$\texttt{beta1} = \texttt{beta10} \cdot \exp\left(\frac{-\texttt{v}}{\texttt{v1}}\right) \tag{5}$$

6.6 Rule 6

Rule is an assignment rule for parameter `beta2`:

$$\texttt{beta2} = \texttt{beta20} \cdot \exp\left(\frac{-\texttt{v}}{\texttt{v2}}\right) \tag{6}$$

6.7 Rule 7

Rule is an assignment rule for parameter `beta3`:

$$\texttt{beta3} = \texttt{beta30} \cdot \exp\left(\frac{-\texttt{v}}{\texttt{v3}}\right) \tag{7}$$

6.8 Rule 8

Rule is an assignment rule for parameter `beta4`:

$$\texttt{beta4} = \texttt{beta40} \cdot \exp\left(\frac{-\texttt{v}}{\texttt{v4}}\right) \tag{8}$$

6.9 Rule 9

Rule is an assignment rule for parameter `I`:

$$\mathtt{I} = (-3.003) \cdot \mathrm{v} \cdot \frac{0.3933 - \exp\left(\frac{-\mathrm{v}}{80.36}\right)}{1 - \exp\left(\frac{\mathrm{v}}{80.36}\right)} \cdot [\mathtt{O}] \tag{9}$$

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 `v0`

Name v0

Trigger The following condition decides whether this trigger may fire:

$$\mathrm{v} = 0 \tag{10}$$

Assignment The values of the assinment formula is computed at the moment this event fires.

$$[\mathrm{v}] = 0.0001 \tag{11}$$

8 Reactions

This model contains eight 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

№	Id	Name	Reaction Equation	SBO
1	re1		C1 ⟶ C2	
2	re2		C2 ⟶ C1	
3	re3		C2 ⟶ C3	
4	re4		C3 ⟶ C2	
5	re7		C3 ⟶ C4	
6	re8		C4 ⟶ C3	
7	re9		C4 ⟶ O	
8	re10		O ⟶ C4	

8.1 Reaction re1

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

Reaction equation

$$\texttt{C1} \longrightarrow \texttt{C2} \tag{12}$$

Reactant

Table 6: Properties of each reactant.

Id	Name	SBO
C1	C1	

Product

Table 7: Properties of each product.

Id	Name	SBO
C2	C2	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \texttt{alpha1} \cdot \texttt{C1} \tag{13}$$

8.2 Reaction re2

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

Reaction equation

$$\texttt{C2} \longrightarrow \texttt{C1} \tag{14}$$

Reactant

Table 8: Properties of each reactant.

Id	Name	SBO
C2	C2	

Product

Table 9: Properties of each product.

Id	Name	SBO
C1	C1	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \texttt{beta1} \cdot [\texttt{C2}] \tag{15}$$

8.3 Reaction re3

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

Reaction equation

$$\texttt{C2} \longrightarrow \texttt{C3} \tag{16}$$

Reactant

Table 10: Properties of each reactant.

Id	Name	SBO
C2	C2	

Product

Table 11: Properties of each product.

Id	Name	SBO
C3	C3	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \texttt{alpha2} \cdot [\texttt{C2}] \tag{17}$$

8.4 Reaction re4

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

Reaction equation

$$\texttt{C3} \longrightarrow \texttt{C2} \tag{18}$$

Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
C3	C3	

Product

Table 13: Properties of each product.

Id	Name	SBO
C2	C2	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \texttt{beta2} \cdot [\texttt{C3}] \tag{19}$$

8.5 Reaction re7

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

Reaction equation

$$\mathtt{C3} \longrightarrow \mathtt{C4} \tag{20}$$

Reactant

Table 14: Properties of each reactant.

Id	Name	SBO
C3	C3	

Product

Table 15: Properties of each product.

Id	Name	SBO
C4	C4	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \mathtt{alpha3} \cdot [\mathtt{C3}] \tag{21}$$

8.6 Reaction re8

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

Reaction equation

$$\mathtt{C4} \longrightarrow \mathtt{C3} \tag{22}$$

Reactant

Table 16: Properties of each reactant.

Id	Name	SBO
C4	C4	

Product

Table 17: Properties of each product.

Id	Name	SBO
C3	C3	

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \texttt{beta3} \cdot [\texttt{C4}] \tag{23}$$

8.7 Reaction re9

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

Reaction equation

$$\texttt{C4} \longrightarrow \texttt{0} \tag{24}$$

Reactant

Table 18: Properties of each reactant.

Id	Name	SBO
C4	C4	

Product

Table 19: Properties of each product.

Id	Name	SBO
O	O	

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \texttt{alpha4} \cdot [\texttt{C4}] \tag{25}$$

8.8 Reaction re10

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

Reaction equation

$$\texttt{O} \longrightarrow \texttt{C4} \tag{26}$$

Reactant

Table 20: Properties of each reactant.

Id	Name	SBO
O	O	

Product

Table 21: Properties of each product.

Id	Name	SBO
C4	C4	

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \texttt{beta4} \cdot [\texttt{O}] \tag{27}$$

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.

9.1 Species C1

Name C1

Initial amount 1 mol

Charge 0

This species takes part in two reactions (as a reactant in re1 and as a product in re2).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathtt{C1} = v_2 - v_1 \tag{28}$$

9.2 Species C2

Name C2

Initial amount 0 mol

This species takes part in four reactions (as a reactant in re2, re3 and as a product in re1, re4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathtt{C2} = v_1 + v_4 - v_2 - v_3 \tag{29}$$

9.3 Species C3

Name C3

Initial amount 0 mol

This species takes part in four reactions (as a reactant in re4, re7 and as a product in re3, re8).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathtt{C3} = v_3 + v_6 - v_4 - v_5 \tag{30}$$

9.4 Species C4

Name C4

Initial amount 0 mol

This species takes part in four reactions (as a reactant in re8, re9 and as a product in re7, re10).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathtt{C4} = v_5 + v_8 - v_6 - v_7 \tag{31}$$

9.5 Species O

Name O

Initial amount 0 mol

This species takes part in two reactions (as a reactant in re10 and as a product in re9).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathsf{O} = v_7 - v_8 \tag{32}$$

9.6 Species v

Name v

Initial amount −70 mol

Charge 0

Involved in event v0

one event influences the species' quantity.

References

Dräger, A., Planatscher, H., Wouamba, D. M., Schröder, A., Hucka, M., Endler, L., Golebiewski, M., Müller, W., and Zell, A. (2009). SBML2LaTeX: Conversion of SBML files into human-readable reports. Bioinformatics, **25**(11), 1455–1456. 10.1093/bioinformatics/btp170.