SBML Model Report

Model name: “Cao2008 - Network of a toggle switch”

May 5, 2016

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by the following two authors: Vijayalakshmi Chelliah[1] and Youfang Cao[2] at September 23rd 2013 at 11:35 a. m. and last time modified at February 24th 2015 at 8:21 p. m. Table 1 provides 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	8
events	0	constraints	0
reactions	8	function definitions	0
global parameters	8	unit definitions	0
rules	0	initial assignments	0

2 Unit Definitions

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

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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
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 eight species. Section 7 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
Pa	Pa	default	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Pb	Pb	default	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Da	Da	default	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Db	Db	default	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
BDa	BDa	default	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
BDb	BDb	default	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
ESA	ESA	default	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
ESB	ESB	default	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟

5 Parameters

This model contains eight global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
da			1.000		☑
db			1.000		☑
sa			100.000		☑
sb			100.000		☑
ba			10^{-5}		☑
bb			10^{-5}		☑
ua			0.100		☑
ub			0.100		☑

6 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 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	re2		$\mathrm{ESA} \xrightarrow{\mathrm{Da,\ Da}} \mathrm{Pa}$	
2	re1		$\mathrm{ESB} \xrightarrow{\mathrm{Db,\ Db}} \mathrm{Pb}$	
3	re12		$\mathrm{Pa} \xrightarrow{\mathrm{Pa}} \mathrm{ESA}$	
4	re11		$\mathrm{Pb} \xrightarrow{\mathrm{Pb}} \mathrm{ESB}$	
5	re13		$2\,\mathrm{Pa} + \mathrm{Db} \xrightarrow{\mathrm{Pa,\ Db}} \mathrm{BDb}$	
6	re5		$2\,\mathrm{Pb} + \mathrm{Da} \xrightarrow{\mathrm{Pb,\ Da}} \mathrm{BDa}$	
7	re7		$\mathrm{BDa} \xrightarrow{\mathrm{BDa}} \mathrm{Da} + 2\,\mathrm{Pb}$	
8	re14		$\mathrm{BDb} \xrightarrow{\mathrm{BDb}} 2\,\mathrm{Pa} + \mathrm{Db}$	

6.1 Reaction re2

This is an irreversible reaction of one reactant forming one product influenced by two modifiers.

Reaction equation

$$\mathrm{ESA} \xrightarrow{\mathrm{Da},\ \mathrm{Da}} \mathrm{Pa} \tag{1}$$

Reactant

Table 6: Properties of each reactant.

Id	Name	SBO
ESA	ESA	

Modifiers

Table 7: Properties of each modifier.

Id	Name	SBO
Da	Da	
Da	Da	

Product

Table 8: Properties of each product.

Id	Name	SBO
Pa	Pa	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \mathrm{vol}\,(\mathrm{default}) \cdot \mathrm{sa} \cdot [\mathrm{Da}] \tag{2}$$

6.2 Reaction re1

This is an irreversible reaction of one reactant forming one product influenced by two modifiers.

Reaction equation

$$\mathrm{ESB} \xrightarrow{\mathrm{Db},\ \mathrm{Db}} \mathrm{Pb} \tag{3}$$

Reactant

Table 9: Properties of each reactant.

Id	Name	SBO
ESB	ESB	

Modifiers

Table 10: Properties of each modifier.

Id	Name	SBO
Db	Db	
Db	Db	

Product

Table 11: Properties of each product.

Id	Name	SBO
Pb	Pb	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \mathrm{vol}\,(\mathrm{default}) \cdot \mathrm{sb} \cdot [\mathrm{Db}] \tag{4}$$

6.3 Reaction re12

This is an irreversible reaction of one reactant forming one product influenced by one modifier.

Reaction equation

$$\mathrm{Pa} \xrightarrow{\mathrm{Pa}} \mathrm{ESA} \tag{5}$$

Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
Pa	Pa	

Modifier

Table 13: Properties of each modifier.

Id	Name	SBO
Pa	Pa	

Product

Table 14: Properties of each product.

Id	Name	SBO
ESA	ESA	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \mathrm{vol}\,(\mathrm{default}) \cdot \mathrm{da} \cdot [\mathrm{Pa}] \tag{6}$$

6.4 Reaction re11

This is an irreversible reaction of one reactant forming one product influenced by one modifier.

Reaction equation

$$\mathrm{Pb} \xrightarrow{\mathrm{Pb}} \mathrm{ESB} \tag{7}$$

Reactant

Table 15: Properties of each reactant.

Id	Name	SBO
Pb	Pb	

Modifier

Table 16: Properties of each modifier.

Id	Name	SBO
Pb	Pb	

Product

Table 17: Properties of each product.

Id	Name	SBO
ESB	ESB	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \mathrm{vol}\,(\mathrm{default}) \cdot \mathrm{db} \cdot [\mathrm{Pb}] \tag{8}$$

6.5 Reaction re13

This is an irreversible reaction of two reactants forming one product influenced by two modifiers.

Reaction equation

$$2\,\mathrm{Pa} + \mathrm{Db} \xrightarrow{\mathrm{Pa,\ Db}} \mathrm{BDb} \tag{9}$$

Reactants

Table 18: Properties of each reactant.

Id	Name	SBO
Pa	Pa	
Db	Db	

Modifiers

Table 19: Properties of each modifier.

Id	Name	SBO
Pa	Pa	
Db	Db	

Product

Table 20: Properties of each product.

Id	Name	SBO
BDb	BDb	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \mathrm{vol}\,(\mathrm{default}) \cdot \mathrm{bb} \cdot \frac{[\mathrm{Pa}] \cdot ([\mathrm{Pa}] - 1)}{2} \cdot [\mathrm{Db}] \tag{10}$$

6.6 Reaction re5

This is an irreversible reaction of two reactants forming one product influenced by two modifiers.

Reaction equation

$$2\,\mathrm{Pb} + \mathrm{Da} \xrightarrow{\mathrm{Pb,\ Da}} \mathrm{BDa} \tag{11}$$

Reactants

Table 21: Properties of each reactant.

Id	Name	SBO
Pb	Pb	
Da	Da	

Modifiers

Table 22: Properties of each modifier.

Id	Name	SBO
Pb	Pb	
Da	Da	

Product

Table 23: Properties of each product.

Id	Name	SBO
BDa	BDa	

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \mathrm{vol}\,(\mathrm{default}) \cdot \mathrm{ba} \cdot \frac{[\mathrm{Pb}] \cdot ([\mathrm{Pb}] - 1)}{2} \cdot [\mathrm{Da}] \tag{12}$$

6.7 Reaction re7

This is an irreversible reaction of one reactant forming two products influenced by one modifier.

Reaction equation

$$\mathrm{BDa} \xrightarrow{\mathrm{BDa}} \mathrm{Da} + 2\,\mathrm{Pb} \tag{13}$$

Reactant

Table 24: Properties of each reactant.

Id	Name	SBO
BDa	BDa	

Modifier

Table 25: Properties of each modifier.

Id	Name	SBO
BDa	BDa	

Products

Table 26: Properties of each product.

Id	Name	SBO
Da	Da	
Pb	Pb	

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \mathrm{vol}\,(\mathrm{default}) \cdot \mathrm{ua} \cdot [\mathrm{BDa}] \tag{14}$$

6.8 Reaction re14

This is an irreversible reaction of one reactant forming two products influenced by one modifier.

Reaction equation

$$\mathrm{BDb} \xrightarrow{\mathrm{BDb}} 2\,\mathrm{Pa} + \mathrm{Db} \tag{15}$$

Reactant

Table 27: Properties of each reactant.

Id	Name	SBO
BDb	BDb	

Modifier

Table 28: Properties of each modifier.

Id	Name	SBO
BDb	BDb	

Products

Table 29: Properties of each product.

Id	Name	SBO
Pa	Pa	
Db	Db	

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \mathrm{vol}\,(\mathrm{default}) \cdot \mathrm{ub} \cdot [\mathrm{BDb}] \tag{16}$$

7 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.

7.1 Species `Pa`

Name Pa

Initial amount 0 mol

Charge 0

This species takes part in six reactions (as a reactant in `re12`, `re13` and as a product in `re2`, `re14` and as a modifier in `re12`, `re13`).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Pa} = v_1 + 2\,v_8 - v_3 - 2\,v_5 \tag{17}$$

7.2 Species `Pb`

Name Pb

Initial amount 0 mol

Charge 0

This species takes part in six reactions (as a reactant in re11, re5 and as a product in re1, re7 and as a modifier in re11, re5).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Pb} = v_2 + 2\,v_7 - v_4 - 2\,v_6 \tag{18}$$

7.3 Species Da

Name Da

Initial amount 0 mol

Charge 0

This species takes part in five reactions (as a reactant in re5 and as a product in re7 and as a modifier in re2, re2, re5).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Da} = v_7 - v_6 \tag{19}$$

7.4 Species Db

Name Db

Initial amount 0 mol

Charge 0

This species takes part in five reactions (as a reactant in re13 and as a product in re14 and as a modifier in re1, re1, re13).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Db} = v_8 - v_5 \tag{20}$$

7.5 Species BDa

Name BDa

Initial amount 0 mol

Charge 0

This species takes part in three reactions (as a reactant in re7 and as a product in re5 and as a modifier in re7).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{BDa} = v_6 - v_7 \tag{21}$$

7.6 Species BDb

Name BDb

Initial amount 0 mol

Charge 0

This species takes part in three reactions (as a reactant in re14 and as a product in re13 and as a modifier in re14).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{BDb} = v_5 - v_8 \tag{22}$$

7.7 Species ESA

Name ESA

SBO:0000291 empty set

Initial amount 0 mol

Charge 0

This species takes part in two reactions (as a reactant in re2 and as a product in re12).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ESA} = v_3 - v_1 \tag{23}$$

7.8 Species ESB

Name ESB

SBO:0000291 empty set

Initial amount 0 mol

Charge 0

This species takes part in two reactions (as a reactant in re1 and as a product in re11).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ESB} = v_4 - v_2 \tag{24}$$

A Glossary of Systems Biology Ontology Terms

SBO:0000291 empty set: Entity defined by the absence of any actual object. An empty set is often used to represent the source of a creation process or the result of a degradation process.

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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