SBML Model Report

Model name: "Cao2013 - Application of ABSIS method in the bistable Schlgl model"

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 12:04 a. m. and last time modified at April fourth 2014 at 4:05 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	1
species types	0	species	2
events	0	constraints	0
reactions	4	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		0000290	3	1	litre	☑	

3.1 Compartment default

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

SBO:0000290 physical compartment

4 Species

This model contains two 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
X	X	default	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
ES	ES	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
k1			3.00		☑
k2			0.60		☑
k3			0.25		☑
k4			2.95		☑
A			1.00		☑
B			2.00		☑
V			25.00		☑
value			1.00		☑

6 Reactions

This model contains four 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	`Reaction1`		$ES \xrightarrow{X,\ X,\ X} X$	
2	`Reaction2`		$X \xrightarrow{X,\ X,\ X} ES$	
3	`Reaction6`		$ES \longrightarrow X$	
4	`Reaction7`		$X \xrightarrow{X} ES$	

6.1 Reaction `Reaction1`

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

Reaction equation

$$\mathrm{ES} \xrightarrow{\mathrm{X},\ \mathrm{X},\ \mathrm{X}} \mathrm{X} \tag{1}$$

Reactant

Table 6: Properties of each reactant.

Id	Name	SBO
ES	ES	

Modifiers

Table 7: Properties of each modifier.

Id	Name	SBO
X	X	
X	X	
X	X	

Product

Table 8: Properties of each product.

Id	Name	SBO
X	X	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \frac{\mathrm{vol\,(default)} \cdot \mathrm{k1} \cdot \mathrm{A} \cdot [\mathrm{X}] \cdot ([\mathrm{X}] - 1)}{\mathrm{V}} \tag{2}$$

6.2 Reaction `Reaction2`

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

Reaction equation

$$\mathrm{X} \xrightarrow{\mathrm{X},\ \mathrm{X},\ \mathrm{X}} \mathrm{ES} \tag{3}$$

Reactant

Table 9: Properties of each reactant.

Id	Name	SBO
X	X	

Modifiers

Table 10: Properties of each modifier.

Id	Name	SBO
X	X	
X	X	
X	X	

Product

Table 11: Properties of each product.

Id	Name	SBO
ES	ES	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \frac{\mathrm{vol}\,(\mathrm{default}) \cdot \frac{\mathrm{k2}}{1} \cdot [\mathrm{X}] \cdot ([\mathrm{X}] - 1) \cdot ([\mathrm{X}] - 2)}{\mathrm{V}^2} \tag{4}$$

6.3 Reaction `Reaction6`

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

Reaction equation

$$\mathrm{ES} \longrightarrow \mathrm{X} \tag{5}$$

Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
ES	ES	

Product

Table 13: Properties of each product.

Id	Name	SBO
X	X	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \mathrm{vol}\,(\mathrm{default}) \cdot \mathrm{k3} \cdot \mathrm{B} \cdot \mathrm{V} \tag{6}$$

6.4 Reaction `Reaction7`

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

Reaction equation

$$\mathrm{X} \xrightarrow{\mathrm{X}} \mathrm{ES} \tag{7}$$

Reactant

Table 14: Properties of each reactant.

Id	Name	SBO
X	X	

Modifier

Table 15: Properties of each modifier.

Id	Name	SBO
X	X	

Id	Name	SBO

Product

Table 16: Properties of each product.

Id	Name	SBO
ES	ES	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \mathrm{vol}\,(\mathrm{default}) \cdot \mathrm{k4} \cdot [\mathrm{X}] \tag{8}$$

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 X

Name X

SBO:0000285 material entity of unspecified nature

Initial amount 1 mol

This species takes part in eleven reactions (as a reactant in Reaction2, Reaction7 and as a product in Reaction1, Reaction6 and as a modifier in Reaction1, Reaction1, Reaction1, Reaction2, Reaction2, Reaction2, Reaction7).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{X} = v_1 + v_3 - v_2 - v_4 \tag{9}$$

7.2 Species ES

Name ES

SBO:0000285 material entity of unspecified nature

Initial amount 1 mol

This species takes part in four reactions (as a reactant in Reaction1, Reaction6 and as a product in Reaction2, Reaction7).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ES} = v_2 + v_4 - v_1 - v_3 \tag{10}$$

A Glossary of Systems Biology Ontology Terms

SBO:0000285 material entity of unspecified nature: Material entity whose nature is unknown or irrelevant

SBO:0000290 physical compartment: Specific location of space, that can be bounded or not. A physical compartment can have 1, 2 or 3 dimensions

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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