SBML Model Report

Model name: “KaDe output:”

August 8, 2017

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	4
events	0	constraints	0
reactions	3	function definitions	0
global parameters	4	unit definitions	2
rules	0	initial assignments	0

2 Unit Definitions

This is an overview of five unit definitions. The units `area`, `length`, and `time` are predefined by SBML and not mentioned in the model.

2.1 Unit `substance`

Name substance

Definition mol

2.2 Unit `volume`

Name volume

Definition l

2.3 Unit `area`

Name Predefined unit area

Notes

Definition m^2

2.4 Unit `length`

Name Predefined unit length

Notes

Definition m

2.5 Unit `time`

Name Predefined unit time

Notes

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 four 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
s1	A(x, y)	default	mol	⊟	⊟
s2	A(x!1, y), A(x!1, y)	default	mol	⊟	⊟
s3	A(x!1, y), A(x, y!1)	default	mol	⊟	⊟
s4	A(x, y!1), A(x, y!1)	default	mol	⊟	⊟

5 Parameters

This model contains four global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
`tinit`			0.00	s	☑
`tend`			1.00	s	☑
`period`			0.01	s	☑
`k`			1.00		☑

6 Reactions

This model contains three 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	A(x,y), A(x,y) -> A(x,y!1), A(x,y!1)	2s1 $\longrightarrow$ 2s4	
2	re2	A(x,y), A(x,y) -> A(x!1,y), A(x,y!1)	2s1 $\longrightarrow$ s3	
3	re3	A(x,y), A(x,y) -> A(x!1,y), A(x!1,y)	2s1 $\longrightarrow$ 2s2	

6.1 Reaction re1

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

Name A(x,y), A(x,y) -> A(x,y!1), A(x,y!1)

Reaction equation

$$2\mathtt{s1} \longrightarrow 2\mathtt{s4} \tag{1}$$

Reactant

Table 6: Properties of each reactant.

Id	Name	SBO
s1	A(x, y)	

Product

Table 7: Properties of each product.

Id	Name	SBO
s4	A(x, y!1), A(x, y!1)	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \frac{\mathtt{k}}{2} \cdot [\mathtt{s1}] \cdot [\mathtt{s1}] \tag{2}$$

6.2 Reaction re2

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

Name A(x,y), A(x,y) -> A(x!1,y), A(x,y!1)

Reaction equation

$$2\mathtt{s1} \longrightarrow \mathtt{s3} \tag{3}$$

Reactant

Table 8: Properties of each reactant.

Id	Name	SBO
s1	A(x, y)	

Product

Table 9: Properties of each product.

Id	Name	SBO
s3	A(x!1, y), A(x, y!1)	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \frac{\mathtt{k}}{2} \cdot [\mathtt{s1}] \cdot [\mathtt{s1}] \tag{4}$$

6.3 Reaction re3

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

Name A(x,y), A(x,y) -> A(x!1,y), A(x!1,y)

Reaction equation

$$2\mathtt{s1} \longrightarrow 2\mathtt{s2} \tag{5}$$

Reactant

Table 10: Properties of each reactant.

Id	Name	SBO
s1	A(x, y)	

Product

Table 11: Properties of each product.

Id	Name	SBO
s2	A(x!1, y), A(x!1, y)	

Id	Name	SBO

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \frac{\mathtt{k}}{2} \cdot [\mathtt{s1}] \cdot [\mathtt{s1}] \tag{6}$$

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 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.

7.1 Species `s1`

Name A(x, y)

Initial amount 100 mol

This species takes part in three reactions (as a reactant in `re1`, `re2`, `re3`).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathtt{s1} = -2\,v_1 - 2\,v_2 - 2\,v_3 \tag{7}$$

7.2 Species `s2`

Name A(x!1, y), A(x!1, y)

Initial amount 0 mol

This species takes part in one reaction (as a product in `re3`).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathtt{s2} = 2\,v_3 \tag{8}$$

7.3 Species s3

Name A(x!1, y), A(x, y!1)

Initial amount 0 mol

This species takes part in one reaction (as a product in re2).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathtt{s3} = v_2 \tag{9}$$

7.4 Species s4

Name A(x, y!1), A(x, y!1)

Initial amount 0 mol

This species takes part in one reaction (as a product in re1).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathtt{s4} = 2\, v_1 \tag{10}$$

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.