SBML Model Report

Model name: "Lee2010_ThrombinActivation-_OneForm_minimal"

May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by Michael Schubert[1] at August 26th 2011 at 4:37 p. m. and last time modified at October nineth 2014 at 5:10 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	4
events	0	constraints	0
reactions	4	function definitions	0
global parameters	0	unit definitions	1
rules	0	initial assignments	0

2 Unit Definitions

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

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2.1 Unit substance

Name substance

Definition µmol

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	compartment		3	1	litre	☑	

3.1 Compartment compartment

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

Name compartment

4 Species

This model contains four species. Section 6 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
II	II	compartment	$\mu mol \cdot l^{-1}$	⊟	⊟
M	M	compartment	$\mu mol \cdot l^{-1}$	⊟	⊟
IIa	IIa	compartment	$\mu mol \cdot l^{-1}$	⊟	⊟
P2	P2	compartment	$\mu mol \cdot l^{-1}$	⊟	⊟

5 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 4: Overview of all reactions

№	Id	Name	Reaction Equation	SBO
1	r1	r1	II $\longrightarrow$ M	
2	r2	r2	M $\longrightarrow$ IIa	
3	r3	r3	II $\longrightarrow$ P2	
4	r4	r4	P2 $\longrightarrow$ IIa	

5.1 Reaction r1

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

Name r1

Reaction equation

$$\mathrm{II} \longrightarrow \mathrm{M} \tag{1}$$

Reactant

Table 5: Properties of each reactant.

Id	Name	SBO
II	II	0000010

Product

Table 6: Properties of each product.

Id	Name	SBO
M	M	0000011

Kinetic Law

SBO:0000049 mass action rate law for first order irreversible reactions, continuous scheme

Derived unit contains undeclared units

$$v_1 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{k1} \cdot [\mathrm{II}] \tag{2}$$

Table 7: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1	0000035	0.005		☑

5.2 Reaction r2

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

Name r2

Reaction equation

$$\mathrm{M} \longrightarrow \mathrm{IIa} \tag{3}$$

Reactant

Table 8: Properties of each reactant.

Id	Name	SBO
M	M	0000010

Product

Table 9: Properties of each product.

Id	Name	SBO
IIa	IIa	0000011

Kinetic Law

SBO:0000049 mass action rate law for first order irreversible reactions, continuous scheme

Derived unit contains undeclared units

$$v_2 = \mathrm{vol}\left(\mathrm{compartment}\right) \cdot \mathrm{k1} \cdot [\mathrm{M}] \tag{4}$$

Table 10: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1	0000035	0.01		☑

5.3 Reaction r3

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

Name r3

Reaction equation

$$\mathrm{II} \longrightarrow \mathrm{P2} \tag{5}$$

Reactant

Table 11: Properties of each reactant.

Id	Name	SBO
II	II	0000010

Product

Table 12: Properties of each product.

Id	Name	SBO
P2	P2	0000011

Kinetic Law

SBO:0000049 mass action rate law for first order irreversible reactions, continuous scheme

Derived unit contains undeclared units

$$v_3 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{k1} \cdot [\mathrm{II}] \tag{6}$$

Table 13: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1	0000035	10^{-5}		☑

5.4 Reaction r4

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

Name r4

Reaction equation

$$\mathrm{P2} \longrightarrow \mathrm{IIa} \tag{7}$$

Reactant

Table 14: Properties of each reactant.

Id	Name	SBO
P2	P2	0000010

Product

Table 15: Properties of each product.

Id	Name	SBO
IIa	IIa	0000011

Kinetic Law

SBO:0000049 mass action rate law for first order irreversible reactions, continuous scheme

Derived unit contains undeclared units

$$v_4 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{k1} \cdot [\mathrm{P2}] \tag{8}$$

Table 16: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1	0000035	$2.5 \cdot 10^{-5}$		☑

6 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.

6.1 Species II

Name II

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

This species takes part in two reactions (as a reactant in r1, r3).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{II} = -v_1 - v_3 \tag{9}$$

6.2 Species M

Name M

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

This species takes part in two reactions (as a reactant in r2 and as a product in r1).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{M} = v_1 - v_2 \tag{10}$$

6.3 Species IIa

Name IIa

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

This species takes part in two reactions (as a product in r2, r4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{IIa} = v_2 + v_4 \tag{11}$$

6.4 Species P2

Name P2

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

This species takes part in two reactions (as a reactant in r4 and as a product in r3).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{P2} = v_3 - v_4 \tag{12}$$

A Glossary of Systems Biology Ontology Terms

SBO:0000010 reactant: Substance consumed by a chemical reaction. Reactants react with each other to form the products of a chemical reaction. In a chemical equation the Reactants are the elements or compounds on the left hand side of the reaction equation. A reactant can be consumed and produced by the same reaction, its global quantity remaining unchanged

SBO:0000011 product: Substance that is produced in a reaction. In a chemical equation the Products are the elements or compounds on the right hand side of the reaction equation. A product can be produced and consumed by the same reaction, its global quantity remaining unchanged

SBO:0000035 forward unimolecular rate constant, continuous case: Numerical parameter that quantifies the forward velocity of a chemical reaction involving only one reactant. This parameter encompasses all the contributions to the velocity except the quantity of the reactant. It is to be used in a reaction modelled using a continuous framework

SBO:0000049 mass action rate law for first order irreversible reactions, continuous scheme: Reaction scheme where the products are created from the reactants and the change of a product quantity is proportional to the product of reactant activities. The reaction scheme does not include any reverse process that creates the reactants from the products. The change of a product quantity is proportional to the quantity of one reactant. It is to be used in a reaction modelled using a continuous framework.

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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