SBML Model Report

Model name: "Lee2010_ThrombinActivation-_OneForm_reduced"

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 4:35 p. m. and last time modified at October nineth 2014 at 4:58 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	9
events	0	constraints	0
reactions	8	function definitions	0
global parameters	12	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.

[1]EBI, schubert@ebi.ac.uk

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 nine 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
E	E	compartment	$\mu mol \cdot l^{-1}$	⊟	⊟
E_P_1	E_P_1	compartment	$\mu mol \cdot l^{-1}$	⊟	⊟
P	P	compartment	$\mu mol \cdot l^{-1}$	⊟	⊟
M	M	compartment	$\mu mol \cdot l^{-1}$	⊟	⊟
E_M	E_M	compartment	$\mu mol \cdot l^{-1}$	⊟	⊟
T	T	compartment	$\mu mol \cdot l^{-1}$	⊟	⊟
E_P_2	E_P_2	compartment	$\mu mol \cdot l^{-1}$	⊟	⊟
P2	P2	compartment	$\mu mol \cdot l^{-1}$	⊟	⊟
E_P2	E_P2	compartment	$\mu mol \cdot l^{-1}$	⊟	⊟

5 Parameters

This model contains twelve global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1	0000036	91.800		☑
k2	k2	0000035	82.400		☑
k3a	k3a	0000036	151.500		☑
k4a	k4a	0000035	209.900		☑
k5	k5	0000036	5.160		☑
k6	k6	0000035	32.300		☑
k7a	k7a	0000036	4.700		☑
k8a	k8a	0000035	42.600		☑
j1	j1	0000038	33.400		☑
j3a	j3a	0000038	0.185		☑
j5	j5	0000038	21.800		☑
j7a	j7a	0000038	$2.66 \cdot 10^{-5}$		☑

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	r1	r1	$E + P \rightleftharpoons E\_P\_1$	
2	r2	r2	$E\_P\_1 \longrightarrow E + M$	
3	r5	r5	$E + M \rightleftharpoons E\_M$	
4	r7	r7	$E\_M \longrightarrow E + T$	
5	r8	r8	$E + P \rightleftharpoons E\_P\_2$	
6	r9	r9	$E\_P\_2 \longrightarrow E + P2$	
7	r12	r12	$E + P2 \rightleftharpoons E\_P2$	
8	r14	r14	$E\_P2 \longrightarrow E + T$	

6.1 Reaction r1

This is a reversible reaction of two reactants forming one product.

Name r1

Reaction equation

$$\mathrm{E} + \mathrm{P} \rightleftharpoons \mathrm{E\_P\_1} \tag{1}$$

Reactants

Table 6: Properties of each reactant.

Id	Name	SBO
E	E	0000010
P	P	0000010

Product

Table 7: Properties of each product.

Id	Name	SBO
E_P_1	E_P_1	0000011

Kinetic Law

SBO:0000101 mass action rate law for second order forward, first order reverse, reversible reactions, two reactants, continuous scheme

Derived unit contains undeclared units

$$v_1 = \mathrm{vol}\,(\mathrm{compartment}) \cdot (\mathrm{k1} \cdot [\mathrm{E}] \cdot [\mathrm{P}] - \mathrm{j1} \cdot [\mathrm{E\_P\_1}]) \tag{2}$$

6.2 Reaction r2

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

Name r2

Reaction equation

$$\mathrm{E\_P\_1} \longrightarrow \mathrm{E} + \mathrm{M} \tag{3}$$

Reactant

Table 8: Properties of each reactant.

Id	Name	SBO
E_P_1	E_P_1	0000010

Products

Table 9: Properties of each product.

Id	Name	SBO
E	E	0000011
M	M	0000011

Kinetic Law

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

Derived unit contains undeclared units

$$v_2 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{k2} \cdot [\mathrm{E\_P\_1}] \tag{4}$$

6.3 Reaction r5

This is a reversible reaction of two reactants forming one product.

Name r5

Reaction equation

$$\mathrm{E} + \mathrm{M} \rightleftharpoons \mathrm{E\_M} \tag{5}$$

Reactants

Table 10: Properties of each reactant.

Id	Name	SBO
E	E	0000010
M	M	0000010

Product

Table 11: Properties of each product.

Id	Name	SBO
E_M	E_M	0000011

Kinetic Law

SBO:0000101 mass action rate law for second order forward, first order reverse, reversible reactions, two reactants, continuous scheme

Derived unit contains undeclared units

$$v_3 = \mathrm{vol}\,(\mathrm{compartment}) \cdot (\mathrm{k3a} \cdot [\mathrm{E}] \cdot [\mathrm{M}] - \mathrm{j3a} \cdot [\mathrm{E\_M}]) \tag{6}$$

6.4 Reaction r7

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

Name r7

Reaction equation

$$\mathrm{E\_M} \longrightarrow \mathrm{E} + \mathrm{T} \tag{7}$$

Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
E_M	E_M	0000010

Products

Table 13: Properties of each product.

Id	Name	SBO
E	E	0000011
T	T	0000011

Kinetic Law

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

Derived unit contains undeclared units

$$v_4 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{k4a} \cdot [\mathrm{E\_M}] \tag{8}$$

6.5 Reaction r8

This is a reversible reaction of two reactants forming one product.

Name r8

Reaction equation

$$\mathrm{E} + \mathrm{P} \rightleftharpoons \mathrm{E\_P\_2} \tag{9}$$

Reactants

Table 14: Properties of each reactant.

Id	Name	SBO
E	E	0000010
P	P	0000010

Product

Table 15: Properties of each product.

Id	Name	SBO
E_P_2	E_P_2	0000011

Kinetic Law

SBO:0000101 mass action rate law for second order forward, first order reverse, reversible reactions, two reactants, continuous scheme

Derived unit contains undeclared units

$$v_5 = \mathrm{vol}\,(\mathrm{compartment}) \cdot (\mathrm{k5} \cdot [\mathrm{E}] \cdot [\mathrm{P}] - \mathrm{j5} \cdot [\mathrm{E\_P\_2}]) \tag{10}$$

6.6 Reaction r9

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

Name r9

Reaction equation

$$\mathrm{E\_P\_2} \longrightarrow \mathrm{E} + \mathrm{P2} \tag{11}$$

Reactant

Table 16: Properties of each reactant.

Id	Name	SBO
E_P_2	E_P_2	0000010

Products

Table 17: Properties of each product.

Id	Name	SBO
E	E	0000011
P2	P2	0000011

Kinetic Law

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

Derived unit contains undeclared units

$$v_6 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{k6} \cdot [\mathrm{E\_P\_2}] \tag{12}$$

6.7 Reaction r12

This is a reversible reaction of two reactants forming one product.

Name r12

Reaction equation

$$\mathrm{E} + \mathrm{P2} \rightleftharpoons \mathrm{E\_P2} \tag{13}$$

Reactants

Table 18: Properties of each reactant.

Id	Name	SBO
E	E	0000010
P2	P2	0000010

Product

Table 19: Properties of each product.

Id	Name	SBO
E_P2	E_P2	0000011

Kinetic Law

SBO:0000101 mass action rate law for second order forward, first order reverse, reversible reactions, two reactants, continuous scheme

Derived unit contains undeclared units

$$v_7 = \mathrm{vol}\,(\mathrm{compartment}) \cdot (\mathrm{k7a} \cdot [\mathrm{E}] \cdot [\mathrm{P2}] - \mathrm{j7a} \cdot [\mathrm{E\_P2}]) \tag{14}$$

6.8 Reaction r14

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

Name r14

Reaction equation

$$\mathrm{E\_P2} \longrightarrow \mathrm{E} + \mathrm{T} \tag{15}$$

Reactant

Table 20: Properties of each reactant.

Id	Name	SBO
E_P2	E_P2	0000010

Products

Table 21: Properties of each product.

Id	Name	SBO
E	E	0000011
T	T	0000011

Kinetic Law

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

Derived unit contains undeclared units

$$v_8 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{k8a} \cdot [\mathrm{E\_P2}] \tag{16}$$

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 E

Name E

Initial concentration $1.5 \cdot 10^{-4}$ µmol $\cdot$ l^{-1}

This species takes part in eight reactions (as a reactant in r1, r5, r8, r12 and as a product in r2, r7, r9, r14).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{E} = v_2 + v_4 + v_6 + v_8 - v_1 - v_3 - v_5 - v_7 \tag{17}$$

7.2 Species E_P_1

Name E_P_1

Initial concentration 0 µmol $\cdot$ l^{-1}

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{E\_P\_1} = v_1 - v_2 \tag{18}$$

7.3 Species P

Name P

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

This species takes part in two reactions (as a reactant in r1, r8).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{P} = -v_1 - v_5 \tag{19}$$

7.4 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 r5 and as a product in r2).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{M} = v_2 - v_3 \tag{20}$$

7.5 Species E_M

Name E_M

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

This species takes part in two reactions (as a reactant in r7 and as a product in r5).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{E\_M} = v_3 - v_4 \tag{21}$$

7.6 Species T

Name T

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

This species takes part in two reactions (as a product in r7, r14).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{T} = v_4 + v_8 \tag{22}$$

7.7 Species E_P_2

Name E_P_2

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

This species takes part in two reactions (as a reactant in r9 and as a product in r8).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{E\_P\_2} = v_5 - v_6 \tag{23}$$

7.8 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 r12 and as a product in r9).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{P2} = v_6 - v_7 \tag{24}$$

7.9 Species E_P2

Name E_P2

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

This species takes part in two reactions (as a reactant in r14 and as a product in r12).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{E\_P2} = v_7 - v_8 \tag{25}$$

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:0000036 forward bimolecular rate constant, continuous case: Numerical parameter that quantifies the forward velocity of a chemical reaction involving two reactants. This parameter encompasses all the contributions to the velocity except the quantity of the reactants. It is to be used in a reaction modelled using a continuous framework

SBO:0000038 reverse unimolecular rate constant, continuous case: Numerical parameter that quantifies the reverse velocity of a chemical reaction involving only one product. This parameter encompasses all the contributions to the velocity except the quantity of the product. 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.

SBO:0000101 mass action rate law for second order forward, first order reverse, reversible reactions, two reactants, 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 include a reverse process that creates the reactants from the products. The rate of the forward process is proportional to the product of two reactant quantities. The rate of the reverse process is proportional to the quantity of one product. 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.

[a]Center for Bioinformatics Tübingen (ZBIT), Germany
[b]California Institute of Technology, Beckman Institute BNMC, Pasadena, United States
[c]European Bioinformatics Institute, Wellcome Trust Genome Campus, Hinxton, United Kingdom
[d]EML Research gGmbH, Heidelberg, Germany