SBML Model Report

Model name: "Panteleev2002-_TFPImechanism_schmema2"

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 4:36 p. m. and last time modified at May 28th 2014 at 4:17 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	9
events	0	constraints	0
reactions	8	function definitions	0
global parameters	0	unit definitions	2
rules	0	initial assignments	0

2 Unit Definitions

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

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2.1 Unit `time`

Name time

Definition 60 s

2.2 Unit `substance`

Name substance

Definition nmol

2.3 Unit `volume`

Notes Litre is the predefined SBML unit for `volume`.

Definition l

2.4 Unit `area`

Notes Square metre is the predefined SBML unit for `area` since SBML Level 2 Version 1.

Definition m^2

2.5 Unit `length`

Notes Metre is the predefined SBML unit for `length` since SBML Level 2 Version 1.

Definition m

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 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
VIIa_TF	VIIa_TF	compartment	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
X	X	compartment	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
VIIa_TF_X	VIIa_TF_X	compartment	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
VIIa_TF_Xa	VIIa_TF_Xa	compartment	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Xa	Xa	compartment	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
TFPI	TFPI	compartment	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Xa_TFPI	Xa_TFPI	compartment	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Xa_TFPI_VIIa_TF	Xa_TFPI_VIIa_TF	compartment	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
VIIa_TF_Xa_TFPI	VIIa_TF_Xa_TFPI	compartment	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟

5 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 4: Overview of all reactions

№	Id	Name	Reaction Equation	SBO
1	reaction_1	reaction_1	$X + VIIa\_TF \rightleftharpoons VIIa\_TF\_X$	
2	reaction_2	reaction_2	$VIIa\_TF\_X \longrightarrow VIIa\_TF\_Xa$	
3	reaction_3	reaction_3	$VIIa\_TF\_Xa \rightleftharpoons Xa + VIIa\_TF$	
4	reaction_4	reaction_4	$Xa + TFPI \rightleftharpoons Xa\_TFPI$	
5	reaction_5	reaction_5	$VIIa\_TF + Xa\_TFPI \rightleftharpoons Xa\_TFPI\_VIIa\_TF$	
6	reaction_6	reaction_6	$VIIa\_TF\_Xa + TFPI \rightleftharpoons VIIa\_TF\_Xa\_TFPI$	
7	reaction_7	reaction_7	$VIIa\_TF\_Xa\_TFPI \rightleftharpoons VIIa\_TF + Xa\_TFPI$	
8	reaction_8	reaction_8	$VIIa\_TF\_Xa\_TFPI \rightleftharpoons Xa\_TFPI\_VIIa\_TF$	

5.1 Reaction `reaction_1`

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

Name reaction_1

Reaction equation

$$\mathrm{X} + \mathrm{VIIa\_TF} \rightleftharpoons \mathrm{VIIa\_TF\_X} \tag{1}$$

Reactants

Table 5: Properties of each reactant.

Id	Name	SBO
`X`	X	0000010
`VIIa_TF`	VIIa_TF	0000010

Product

Table 6: Properties of each product.

Id	Name	SBO
`VIIa_TF_X`	VIIa_TF_X	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

$$v_1 = \mathrm{vol}\,(\mathrm{compartment}) \cdot (\mathrm{k1} \cdot [\mathrm{X}] \cdot [\mathrm{VIIa\_TF}] - \mathrm{k2} \cdot [\mathrm{VIIa\_TF\_X}]) \tag{2}$$

Table 7: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
`k1`	k1	0000036	5.0		☑
`k2`	k2	0000038	770.0		☑

5.2 Reaction reaction_2

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

Name reaction_2

Reaction equation

$$\text{VIIa\_TF\_X} \longrightarrow \text{VIIa\_TF\_Xa} \tag{3}$$

Reactant

Table 8: Properties of each reactant.

Id	Name	SBO
VIIa_TF_X	VIIa_TF_X	0000010

Product

Table 9: Properties of each product.

Id	Name	SBO
VIIa_TF_Xa	VIIa_TF_Xa	0000011

Kinetic Law

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

Derived unit contains undeclared units

$$v_2 = \text{vol}\,(\text{compartment}) \cdot \text{k1} \cdot [\text{VIIa\_TF\_X}] \tag{4}$$

Table 10: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1	0000035	420.0		☑

5.3 Reaction reaction_3

This is a reversible reaction of one reactant forming two products.

Name reaction_3

Reaction equation

$$\text{VIIa\_TF\_Xa} \rightleftharpoons \text{Xa} + \text{VIIa\_TF} \tag{5}$$

Reactant

Table 11: Properties of each reactant.

Id	Name	SBO
VIIa_TF_Xa	VIIa_TF_Xa	0000010

Products

Table 12: Properties of each product.

Id	Name	SBO
Xa	Xa	0000011
VIIa_TF	VIIa_TF	0000011

Kinetic Law

SBO:0000083 mass action rate law for first order forward, second order reverse, reversible reactions, two products, continuous scheme

Derived unit contains undeclared units

$$v_3 = \text{vol}\,(\text{compartment}) \cdot (\text{k1} \cdot [\text{VIIa\_TF\_Xa}] - \text{k2} \cdot [\text{Xa}] \cdot [\text{VIIa\_TF}]) \tag{6}$$

Table 13: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1	0000035	770.0		☑
k2	k2	0000039	5.0		☑

5.4 Reaction reaction_4

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

Name reaction_4

Reaction equation

$$\mathrm{Xa} + \mathrm{TFPI} \rightleftharpoons \mathrm{Xa\_TFPI} \tag{7}$$

Reactants

Table 14: Properties of each reactant.

Id	Name	SBO
Xa	Xa	0000010
TFPI	TFPI	0000010

Product

Table 15: Properties of each product.

Id	Name	SBO
Xa_TFPI	Xa_TFPI	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

$$v_4 = \mathrm{vol}\,(\mathrm{compartment}) \cdot (\mathrm{k1} \cdot [\mathrm{Xa}] \cdot [\mathrm{TFPI}] - \mathrm{k2} \cdot [\mathrm{Xa\_TFPI}]) \tag{8}$$

Table 16: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1	0000036	0.054		☑
k2	k2	0000038	0.020		☑

5.5 Reaction reaction_5

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

Name reaction_5

Reaction equation

$$\mathrm{VIIa\_TF} + \mathrm{Xa\_TFPI} \rightleftharpoons \mathrm{Xa\_TFPI\_VIIa\_TF} \tag{9}$$

Reactants

Table 17: Properties of each reactant.

Id	Name	SBO
VIIa_TF	VIIa_TF	0000010
Xa_TFPI	Xa_TFPI	0000010

Product

Table 18: Properties of each product.

Id	Name	SBO
Xa_TFPI_VIIa_TF	Xa_TFPI_VIIa_TF	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

$$v_5 = \mathrm{vol}\,(\mathrm{compartment}) \cdot (\mathrm{k1} \cdot [\mathrm{VIIa\_TF}] \cdot [\mathrm{Xa\_TFPI}] - \mathrm{k2} \cdot [\mathrm{Xa\_TFPI\_VIIa\_TF}]) \tag{10}$$

Table 19: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1	0000036	0.440		☑
k2	k2	0000038	0.066		☑

5.6 Reaction reaction_6

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

Name reaction_6

Reaction equation

$$\mathrm{VIIa\_TF\_Xa} + \mathrm{TFPI} \rightleftharpoons \mathrm{VIIa\_TF\_Xa\_TFPI} \tag{11}$$

Reactants

Table 20: Properties of each reactant.

Id	Name	SBO
VIIa_TF_Xa	VIIa_TF_Xa	0000010
TFPI	TFPI	0000010

Product

Table 21: Properties of each product.

Id	Name	SBO
VIIa_TF_Xa_TFPI	VIIa_TF_Xa_TFPI	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

$$v_6 = \mathrm{vol}\,(\mathrm{compartment}) \cdot (\mathrm{k1} \cdot [\mathrm{VIIa\_TF\_Xa}] \cdot [\mathrm{TFPI}] - \mathrm{k2} \cdot [\mathrm{VIIa\_TF\_Xa\_TFPI}]) \tag{12}$$

Table 22: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1	0000036	10.0		☑
k2	k2	0000038	0.0		☑

5.7 Reaction reaction_7

This is a reversible reaction of one reactant forming two products.

Name reaction_7

Reaction equation

$$\text{VIIa\_TF\_Xa\_TFPI} \rightleftharpoons \text{VIIa\_TF} + \text{Xa\_TFPI} \tag{13}$$

Reactant

Table 23: Properties of each reactant.

Id	Name	SBO
VIIa_TF_Xa_TFPI	VIIa_TF_Xa_TFPI	0000010

Products

Table 24: Properties of each product.

Id	Name	SBO
VIIa_TF	VIIa_TF	0000011
Xa_TFPI	Xa_TFPI	0000011

Kinetic Law

SBO:0000083 mass action rate law for first order forward, second order reverse, reversible reactions, two products, continuous scheme

Derived unit contains undeclared units

$$v_7 = \text{vol}(\text{compartment}) \cdot (\text{k1} \cdot [\text{VIIa\_TF\_Xa\_TFPI}] - \text{k2} \cdot [\text{VIIa\_TF}] \cdot [\text{Xa\_TFPI}]) \tag{14}$$

Table 25: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1	0000035	0.0		☑
k2	k2	0000039	0.0		☑

5.8 Reaction reaction_8

This is a reversible reaction of one reactant forming one product.

Name reaction_8

Reaction equation

$$\text{VIIa\_TF\_Xa\_TFPI} \rightleftharpoons \text{Xa\_TFPI\_VIIa\_TF} \tag{15}$$

Reactant

Table 26: Properties of each reactant.

Id	Name	SBO
VIIa_TF_Xa_TFPI	VIIa_TF_Xa_TFPI	0000010

Product

Table 27: Properties of each product.

Id	Name	SBO
Xa_TFPI_VIIa_TF	Xa_TFPI_VIIa_TF	0000011

Kinetic Law

SBO:0000080 mass action rate law for first order forward, first order reverse, reversible reactions, continuous scheme

Derived unit contains undeclared units

$$v_8 = \text{vol}\,(\text{compartment}) \cdot (\text{k1} \cdot [\text{VIIa\_TF\_Xa\_TFPI}] - \text{k2} \cdot [\text{Xa\_TFPI\_VIIa\_TF}]) \tag{16}$$

Table 28: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1	0000035	0.0		☑
k2	k2	0000038	0.0		☑

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 `VIIa_TF`

Name VIIa_TF

Initial concentration $0.9999997\ \mathrm{nmol} \cdot \mathrm{l}^{-1}$

This species takes part in four reactions (as a reactant in `reaction_1`, `reaction_5` and as a product in `reaction_3`, `reaction_7`).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{VIIa\_TF} = v_3 + v_7 - v_1 - v_5 \tag{17}$$

6.2 Species `X`

Name X

Initial concentration $169.9999\ \mathrm{nmol} \cdot \mathrm{l}^{-1}$

This species takes part in one reaction (as a reactant in `reaction_1`).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{X} = -v_1 \tag{18}$$

6.3 Species `VIIa_TF_X`

Name VIIa_TF_X

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

This species takes part in two reactions (as a reactant in `reaction_2` and as a product in `reaction_1`).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{VIIa\_TF\_X} = v_1 - v_2 \tag{19}$$

6.4 Species `VIIa_TF_Xa`

Name VIIa_TF_Xa

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

This species takes part in three reactions (as a reactant in `reaction_3`, `reaction_6` and as a product in `reaction_2`).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{VIIa\_TF\_Xa} = v_2 - v_3 - v_6 \tag{20}$$

6.5 Species Xa

Name Xa

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

This species takes part in two reactions (as a reactant in reaction_4 and as a product in reaction_3).

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

6.6 Species TFPI

Name TFPI

Initial concentration $2.399999\ \mathrm{nmol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in reaction_4, reaction_6).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{TFPI} = -v_4 - v_6 \tag{22}$$

6.7 Species Xa_TFPI

Name Xa_TFPI

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

This species takes part in three reactions (as a reactant in reaction_5 and as a product in reaction_4, reaction_7).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Xa\_TFPI} = v_4 + v_7 - v_5 \tag{23}$$

6.8 Species Xa_TFPI_VIIa_TF

Name Xa_TFPI_VIIa_TF

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

This species takes part in two reactions (as a product in reaction_5, reaction_8).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Xa\_TFPI\_VIIa\_TF} = v_5 + v_8 \tag{24}$$

6.9 Species VIIa_TF_Xa_TFPI

Name VIIa_TF_Xa_TFPI

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

This species takes part in three reactions (as a reactant in reaction_7, reaction_8 and as a product in reaction_6).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{VIIa\_TF\_Xa\_TFPI} = v_6 - v_7 - v_8 \tag{25}$$

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:0000039 reverse bimolecular 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:0000080 mass action rate law for first order forward, first order reverse, reversible 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 include a reverse process that creates the reactants from the products. The rate of the forward process is proportional to the quantity of one reactant. 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.

SBO:0000083 mass action rate law for first order forward, second order reverse, reversible reactions, two products, 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 quantity of one reactant. The rate of the reverse process is proportional to the product of two product quantities. 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.

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