Model name: “Stortelder1997 - Thrombin Generation Amidolytic Activity”

May 5, 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 26\(^{th}\) 2011 at 4:35 p.m. and last time modified at October nineth 2014 at 5:03 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.

<table>
<thead>
<tr>
<th>Element</th>
<th>Quantity</th>
<th>Element</th>
<th>Quantity</th>
</tr>
</thead>
<tbody>
<tr>
<td>compartment types</td>
<td>0</td>
<td>compartments</td>
<td>1</td>
</tr>
<tr>
<td>species types</td>
<td>0</td>
<td>species</td>
<td>12</td>
</tr>
<tr>
<td>events</td>
<td>0</td>
<td>constraints</td>
<td>0</td>
</tr>
<tr>
<td>reactions</td>
<td>8</td>
<td>function definitions</td>
<td>1</td>
</tr>
<tr>
<td>global parameters</td>
<td>14</td>
<td>unit definitions</td>
<td>2</td>
</tr>
<tr>
<td>rules</td>
<td>1</td>
<td>initial assignments</td>
<td>0</td>
</tr>
</tbody>
</table>

**Model Notes**

Stortelder1997 - Thrombin Generation Amidolytic Activity

Mathematical modelling of a part of the blood coagulation mechanism.


\(^1\)EBI, schubert@ebi.ac.uk
Abstract:

This paper describes the mathematical modelling of a part of the blood coagulation mechanism. The model includes the activation of factor X by a purified enzyme from Russel’s Viper Venom (RVV), factor V and prothrombin, and also comprises the inactivation of the products formed. In this study we assume that in principle the mechanism of the process is known. However, the exact structure of the mechanism is unknown, and the process still can be described by different mathematical models. These models are put to test by measuring their capacity to explain the course of thrombin generation as observed in plasma after recalcification in presence of RVV. The mechanism studied is mathematically modelled as a system of differential-algebraic equations (DAEs). Each candidate model contains some freedom, which is expressed in the model equations by the presence of unknown parameters. For example, reaction constants or initial concentrations are unknown. The goal of parameter estimation is to determine these unknown parameters in such a way that the theoretical (i.e., computed) results fit the experimental data within measurement accuracy and to judge which modifications of the chemical reaction scheme allow the best fit. We present results on model discrimination and estimation of reaction constants, which are hard to obtain in another way.

This model is hosted on BioModels Database and identified by: BIOMD0000000358.

To cite BioModels Database, please use: BioModels Database: An enhanced, curated and annotated resource for published quantitative kinetic models.

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2 Unit Definitions

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

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>
<thead>
<tr>
<th>Id</th>
<th>Name</th>
<th>SBO</th>
<th>Spatial Dimensions</th>
<th>Size</th>
<th>Unit</th>
<th>Constant</th>
<th>Outside</th>
</tr>
</thead>
<tbody>
<tr>
<td>compartment_1</td>
<td>compartment_1</td>
<td></td>
<td></td>
<td>3</td>
<td>litre</td>
<td>✓</td>
<td></td>
</tr>
</tbody>
</table>

3.1 Compartment compartment_1

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

Name compartment_1
4 Species

This model contains twelve species. Section 9 provides further details and the derived rates of change of each species.

Table 3: Properties of each species.

<table>
<thead>
<tr>
<th>Id</th>
<th>Name</th>
<th>Compartment</th>
<th>Derived Unit</th>
<th>Constant</th>
<th>Boundary Condition</th>
</tr>
</thead>
<tbody>
<tr>
<td>X</td>
<td>X</td>
<td>compartment_1</td>
<td>nmol·l⁻¹</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Xa</td>
<td>Xa</td>
<td>compartment_1</td>
<td>nmol·l⁻¹</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Xa_ATIII</td>
<td>Xa_ATIII</td>
<td>compartment_1</td>
<td>nmol·l⁻¹</td>
<td></td>
<td></td>
</tr>
<tr>
<td>PL</td>
<td>PL</td>
<td>compartment_1</td>
<td>nmol·l⁻¹</td>
<td></td>
<td></td>
</tr>
<tr>
<td>PT</td>
<td>PT</td>
<td>compartment_1</td>
<td>nmol·l⁻¹</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Va</td>
<td>Va</td>
<td>compartment_1</td>
<td>nmol·l⁻¹</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ila</td>
<td>Ila</td>
<td>compartment_1</td>
<td>nmol·l⁻¹</td>
<td></td>
<td></td>
</tr>
<tr>
<td>V</td>
<td>V</td>
<td>compartment_1</td>
<td>nmol·l⁻¹</td>
<td></td>
<td></td>
</tr>
<tr>
<td>II</td>
<td>II</td>
<td>compartment_1</td>
<td>nmol·l⁻¹</td>
<td></td>
<td></td>
</tr>
<tr>
<td>IIa_alpha2M</td>
<td>IIa_alpha2M</td>
<td>compartment_1</td>
<td>nmol·l⁻¹</td>
<td></td>
<td></td>
</tr>
<tr>
<td>IIa_ATIII</td>
<td>IIa_ATIII</td>
<td>compartment_1</td>
<td>nmol·l⁻¹</td>
<td></td>
<td></td>
</tr>
<tr>
<td>RVV</td>
<td>RVV</td>
<td>compartment_1</td>
<td>nmol·l⁻¹</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
5 Parameters

This model contains 14 global parameters.

<table>
<thead>
<tr>
<th>Id</th>
<th>Name</th>
<th>SBO</th>
<th>Value</th>
<th>Unit</th>
<th>Constant</th>
</tr>
</thead>
<tbody>
<tr>
<td>kcat_X</td>
<td>kcat_X</td>
<td>0000025</td>
<td>239.100</td>
<td>unit</td>
<td></td>
</tr>
<tr>
<td>km_X</td>
<td>km_X</td>
<td>0000371</td>
<td>23.650</td>
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<td></td>
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<tr>
<td>ki_Xa</td>
<td>ki_Xa</td>
<td>0000035</td>
<td>4.531</td>
<td></td>
<td></td>
</tr>
<tr>
<td>k_PT</td>
<td>k_PT</td>
<td>0000037</td>
<td>122.900</td>
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<td></td>
</tr>
<tr>
<td>k_PL</td>
<td>k_PL</td>
<td>0000038</td>
<td>801.400</td>
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<td></td>
</tr>
<tr>
<td>kcat_V</td>
<td>kcat_V</td>
<td>0000025</td>
<td>7.844</td>
<td></td>
<td></td>
</tr>
<tr>
<td>km_V</td>
<td>km_V</td>
<td>0000371</td>
<td>149.700</td>
<td></td>
<td></td>
</tr>
<tr>
<td>kcat_II</td>
<td>kcat_II</td>
<td>0000025</td>
<td>43.870</td>
<td></td>
<td></td>
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<td>km_II</td>
<td>km_II</td>
<td>0000371</td>
<td>62.250</td>
<td></td>
<td></td>
</tr>
<tr>
<td>kcat_2</td>
<td>kcat_2</td>
<td>0000025</td>
<td>12.400</td>
<td></td>
<td></td>
</tr>
<tr>
<td>km_2</td>
<td>km_2</td>
<td>0000371</td>
<td>0.061</td>
<td></td>
<td></td>
</tr>
<tr>
<td>ki_IIaAlpha2M</td>
<td>ki_IIaAlpha2M</td>
<td>00000035</td>
<td>0.176</td>
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<td></td>
</tr>
<tr>
<td>ki_IIaATIII</td>
<td>ki_IIaATIII</td>
<td>00000035</td>
<td>0.786</td>
<td></td>
<td></td>
</tr>
<tr>
<td>AmAct</td>
<td>AmAct</td>
<td>0.000</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

6 Function definition

This is an overview of one function definition.

6.1 Function definition HenriMichaelisMenten_irreversible_kcat

Name Henri-Michaelis-Menten (irreversible) kcat

Arguments kcat, enzyme, substrate, Km

Mathematical Expression

\[
\frac{kcat \cdot enzyme \cdot substrate}{Km + substrate}
\]  

7 Rule

This is an overview of one rule.
7.1 Rule AmAct

Rule AmAct is an assignment rule for parameter AmAct:

\[
\text{AmAct} = [\text{IIa}] + 0.556 \cdot [\text{IIa}_{\text{alpha}2M}]
\]  \hspace{1cm} (2)
8 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

<table>
<thead>
<tr>
<th>№</th>
<th>Id</th>
<th>Name</th>
<th>Reaction Equation</th>
<th>SBO</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>R1</td>
<td>R1</td>
<td>$X \xrightarrow{RVV} X_a$</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>R2</td>
<td>R2</td>
<td>$X_a \rightarrow X_a_ATIII$</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>R3</td>
<td>R3</td>
<td>$V_a + X_a + PL \rightleftharpoons PT$</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>R4</td>
<td>R4</td>
<td>$V \rightleftharpoons V_a$</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>R5</td>
<td>R5</td>
<td>$II \xrightarrow{PT} IIa$</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>R6</td>
<td>R6</td>
<td>$II \xrightarrow{X_a} IIa$</td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>R7</td>
<td>R7</td>
<td>$IIa \rightarrow IIa_alpha2M$</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>R8</td>
<td>R8</td>
<td>$IIa \rightarrow IIa_ATIII$</td>
<td></td>
</tr>
</tbody>
</table>
8.1 Reaction $R_1$

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

**Name** $R_1$

**Reaction equation**

$$X \xrightarrow{RVV} X_a \quad (3)$$

**Reactant**

Table 6: Properties of each reactant.

<table>
<thead>
<tr>
<th>Id</th>
<th>Name</th>
<th>SBO</th>
</tr>
</thead>
<tbody>
<tr>
<td>X</td>
<td>X</td>
<td>0000010</td>
</tr>
</tbody>
</table>

**Modifier**

Table 7: Properties of each modifier.

<table>
<thead>
<tr>
<th>Id</th>
<th>Name</th>
<th>SBO</th>
</tr>
</thead>
<tbody>
<tr>
<td>RVV</td>
<td>RVV</td>
<td>0000461</td>
</tr>
</tbody>
</table>

**Product**

Table 8: Properties of each product.

<table>
<thead>
<tr>
<th>Id</th>
<th>Name</th>
<th>SBO</th>
</tr>
</thead>
<tbody>
<tr>
<td>Xa</td>
<td>Xa</td>
<td>0000011</td>
</tr>
</tbody>
</table>

**Kinetic Law**

**SBO:0000028** enzymatic rate law for irreversible non-modulated non-interacting unireactant enzymes

**Derived unit** contains undeclared units

$$v_1 = \text{vol (compartment}_1) \cdot \text{HenriMichaelisMenten_irreversible}_{kat}(kcat_X, [RVV], [X], km_X) \quad (4)$$
\[
\text{HenriMichaelisMenten\_irreversible\_kcat (kcat, enzyme, substrate, Km)}
\]
\[
= \frac{\text{kcat} \cdot \text{enzyme} \cdot \text{substrate}}{\text{Km} + \text{substrate}}
\]  

\[
\text{HenriMichaelisMenten\_irreversible\_kcat (kcat, enzyme, substrate, Km)}
\]
\[
= \frac{\text{kcat} \cdot \text{enzyme} \cdot \text{substrate}}{\text{Km} + \text{substrate}}
\]  

### 8.2 Reaction R2

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

**Name** R2

**Reaction equation**

\[Xa \rightarrow Xa_{ATIII}\]  

**Reactant**

<table>
<thead>
<tr>
<th>Id</th>
<th>Name</th>
<th>SBO</th>
</tr>
</thead>
<tbody>
<tr>
<td>Xa</td>
<td>Xa</td>
<td>0000010</td>
</tr>
</tbody>
</table>

**Product**

<table>
<thead>
<tr>
<th>Id</th>
<th>Name</th>
<th>SBO</th>
</tr>
</thead>
<tbody>
<tr>
<td>Xa_ATIII</td>
<td>Xa_ATIII</td>
<td>0000011</td>
</tr>
</tbody>
</table>

**Kinetic Law**

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

**Derived unit** contains undeclared units

\[v_2 = \text{vol (compartment\_1)} \cdot \text{ki\_Xa} \cdot [Xa]\]  

### 8.3 Reaction R3

This is a reversible reaction of three reactants forming one product.
Name R3

Reaction equation

\[ \text{Va} + \text{Xa} + \text{PL} \rightleftharpoons \text{PT} \]  \hspace{1cm} (9)

Reactants

Table 11: Properties of each reactant.

<table>
<thead>
<tr>
<th>Id</th>
<th>Name</th>
<th>SBO</th>
</tr>
</thead>
<tbody>
<tr>
<td>Va</td>
<td>Va</td>
<td>000010</td>
</tr>
<tr>
<td>Xa</td>
<td>Xa</td>
<td>000010</td>
</tr>
<tr>
<td>PL</td>
<td>PL</td>
<td>000010</td>
</tr>
</tbody>
</table>

Product

Table 12: Properties of each product.

<table>
<thead>
<tr>
<th>Id</th>
<th>Name</th>
<th>SBO</th>
</tr>
</thead>
<tbody>
<tr>
<td>PT</td>
<td>PT</td>
<td>000011</td>
</tr>
</tbody>
</table>

Kinetic Law

SBO:0000122 mass action rate law for third order forward, first order reverse, reversible reactions, three reactants, continuous scheme

Derived unit contains undeclared units

\[ v_3 = \text{vol (compartment}_1\text{)} \cdot (k_{PT} \cdot [\text{Va}] \cdot [\text{Xa}] \cdot [\text{PL}] - k_{PL} \cdot [\text{PT}]) \]  \hspace{1cm} (10)

8.4 Reaction R4

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

Name R4

Reaction equation

\[ \text{V} \xrightarrow{Ia} \text{Va} \]  \hspace{1cm} (11)

Reactant
**Table 13: Properties of each reactant.**

<table>
<thead>
<tr>
<th>Id</th>
<th>Name</th>
<th>SBO</th>
</tr>
</thead>
<tbody>
<tr>
<td>V</td>
<td>V</td>
<td>0000010</td>
</tr>
</tbody>
</table>

**Modifier**

**Table 14: Properties of each modifier.**

<table>
<thead>
<tr>
<th>Id</th>
<th>Name</th>
<th>SBO</th>
</tr>
</thead>
<tbody>
<tr>
<td>IIa</td>
<td>IIa</td>
<td>0000461</td>
</tr>
</tbody>
</table>

**Product**

**Table 15: Properties of each product.**

<table>
<thead>
<tr>
<th>Id</th>
<th>Name</th>
<th>SBO</th>
</tr>
</thead>
<tbody>
<tr>
<td>Va</td>
<td>Va</td>
<td>0000011</td>
</tr>
</tbody>
</table>

**Kinetic Law**

**SBO:0000028** enzymatic rate law for irreversible non-modulated non-interacting unireactant enzymes

**Derived unit** contains undeclared units

\[

v_4 = \text{vol} (\text{compartment}_1) \cdot \text{HenriMichaelisMenten_irreversible_kcat} (k\text{cat}, [\text{IIa}], [V], \text{km}_V)

\]

(12)

\[

\text{HenriMichaelisMenten_irreversible_kcat} (k\text{cat}, \text{enzyme, substrate, Km}) = \frac{k\text{cat} \cdot \text{enzyme} \cdot \text{substrate}}{\text{Km} + \text{substrate}}

\]

(13)

\[

\text{HenriMichaelisMenten_irreversible_kcat} (k\text{cat}, \text{enzyme, substrate, Km}) = \frac{k\text{cat} \cdot \text{enzyme} \cdot \text{substrate}}{\text{Km} + \text{substrate}}

\]

(14)

**8.5 Reaction** **R5**

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

**Name** **R5**
Reaction equation

II $\rightarrow$ IIa  \hspace{1cm} (15)

Reactant

Table 16: Properties of each reactant.

<table>
<thead>
<tr>
<th>Id</th>
<th>Name</th>
<th>SBO</th>
</tr>
</thead>
<tbody>
<tr>
<td>II</td>
<td>II</td>
<td>0000010</td>
</tr>
</tbody>
</table>

Modifier

Table 17: Properties of each modifier.

<table>
<thead>
<tr>
<th>Id</th>
<th>Name</th>
<th>SBO</th>
</tr>
</thead>
<tbody>
<tr>
<td>PT</td>
<td>PT</td>
<td>0000461</td>
</tr>
</tbody>
</table>

Product

Table 18: Properties of each product.

<table>
<thead>
<tr>
<th>Id</th>
<th>Name</th>
<th>SBO</th>
</tr>
</thead>
<tbody>
<tr>
<td>IIa</td>
<td>IIa</td>
<td>0000011</td>
</tr>
</tbody>
</table>

Kinetic Law

**SBO:0000028** enzymatic rate law for irreversible non-modulated non-interacting unireactant enzymes

**Derived unit** contains undeclared units

\[ v_5 = \text{vol (compartment,1) } \cdot \text{HenriMichaelisMenten_irreversible_kcat (kcat,II,[PT],[II],km,II)} \]  \hspace{1cm} (16)

\[ \text{HenriMichaelisMenten_irreversible_kcat (kcat,enzyme,substrate,Km)} = \frac{kcat \cdot \text{enzyme} \cdot \text{substrate}}{Km + \text{substrate}} \]  \hspace{1cm} (17)

\[ \text{HenriMichaelisMenten_irreversible_kcat (kcat,enzyme,substrate,Km)} = \frac{kcat \cdot \text{enzyme} \cdot \text{substrate}}{Km + \text{substrate}} \]  \hspace{1cm} (18)
8.6 Reaction R6

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

**Name** R6

**Reaction equation**

\[
\text{II} \xrightarrow{Xa} \text{IIa} \quad (19)
\]

**Reactant**

Table 19: Properties of each reactant.

<table>
<thead>
<tr>
<th>Id</th>
<th>Name</th>
<th>SBO</th>
</tr>
</thead>
<tbody>
<tr>
<td>II</td>
<td>II</td>
<td>0000010</td>
</tr>
</tbody>
</table>

**Modifier**

Table 20: Properties of each modifier.

<table>
<thead>
<tr>
<th>Id</th>
<th>Name</th>
<th>SBO</th>
</tr>
</thead>
<tbody>
<tr>
<td>Xa</td>
<td>Xa</td>
<td>0000461</td>
</tr>
</tbody>
</table>

**Product**

Table 21: Properties of each product.

<table>
<thead>
<tr>
<th>Id</th>
<th>Name</th>
<th>SBO</th>
</tr>
</thead>
<tbody>
<tr>
<td>IIa</td>
<td>IIa</td>
<td>0000011</td>
</tr>
</tbody>
</table>

**Kinetic Law**

*SBO:0000028* enzymatic rate law for irreversible non-modulated non-interacting unireactant enzymes

**Derived unit** contains undeclared units

\[
v_6 = \text{vol (compartment}_1) \cdot \text{HenriMichaelisMenten_irreversible}_\text{kcat (kcat}_2, [Xa], [II], \text{km}_2) \quad (20)
\]
HenriMichaelisMenten_irreversible_kcat (kcat, enzyme, substrate, Km) = \frac{kcat \cdot enzyme \cdot substrate}{Km + substrate} \tag{21}

HenriMichaelisMenten_irreversible_kcat (kcat, enzyme, substrate, Km) = \frac{kcat \cdot enzyme \cdot substrate}{Km + substrate} \tag{22}

8.7 Reaction R7
This is an irreversible reaction of one reactant forming one product.

Name R7

Reaction equation
\[\text{IIa} \rightarrow \text{IIa}_\text{alpha2M}\] \tag{23}

Reactant

Table 22: Properties of each reactant.

<table>
<thead>
<tr>
<th>Id</th>
<th>Name</th>
<th>SBO</th>
</tr>
</thead>
<tbody>
<tr>
<td>IIa</td>
<td>IIa</td>
<td>0000010</td>
</tr>
</tbody>
</table>

Product

Table 23: Properties of each product.

<table>
<thead>
<tr>
<th>Id</th>
<th>Name</th>
<th>SBO</th>
</tr>
</thead>
<tbody>
<tr>
<td>IIa_alpha2M</td>
<td>IIa_alpha2M</td>
<td>0000011</td>
</tr>
</tbody>
</table>

Kinetic Law

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

Derived unit contains undeclared units

\[v_7 = \text{vol (compartment}_1) \cdot ki_{\text{IIaAlpha2M}} \cdot [\text{IIa}]\] \tag{24}

8.8 Reaction R8
This is an irreversible reaction of one reactant forming one product.
Name R8

Reaction equation

\[ \text{IIa} \rightarrow \text{IIa_ATIII} \quad (25) \]

Reactant

Table 24: Properties of each reactant.

<table>
<thead>
<tr>
<th>Id</th>
<th>Name</th>
<th>SBO</th>
</tr>
</thead>
<tbody>
<tr>
<td>IIa</td>
<td>IIa</td>
<td>0000010</td>
</tr>
</tbody>
</table>

Product

Table 25: Properties of each product.

<table>
<thead>
<tr>
<th>Id</th>
<th>Name</th>
<th>SBO</th>
</tr>
</thead>
<tbody>
<tr>
<td>IIa_ATIII</td>
<td>IIa_ATIII</td>
<td>0000011</td>
</tr>
</tbody>
</table>

Kinetic Law

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

Derived unit contains undeclared units

\[ v_8 = \text{vol(compartment}_1) \cdot \text{ki}_{\text{IIa_ATIII}} \cdot [\text{IIa}] \quad (26) \]

9 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.
### 9.1 Species X

**Name** X  
**Initial concentration** 81.24998 nmol·l⁻¹  
This species takes part in one reaction (as a reactant in R1).

\[
\frac{d}{dt}X = -v_1  
\tag{27}
\]

### 9.2 Species Xa

**Name** Xa  
**Initial concentration** 0 nmol·l⁻¹  
This species takes part in four reactions (as a reactant in R2, R3 and as a product in R1 and as a modifier in R6).

\[
\frac{d}{dt}X_a = v_1 - v_2 - v_3  
\tag{28}
\]

### 9.3 Species Xa_ATIII

**Name** Xa_ATIII  
**Initial concentration** 0 nmol·l⁻¹  
This species takes part in one reaction (as a product in R2).

\[
\frac{d}{dt}X_a_ATIII = v_2  
\tag{29}
\]

### 9.4 Species PL

**Name** PL  
**Initial concentration** 9.999997 nmol·l⁻¹  
This species takes part in one reaction (as a reactant in R3).

\[
\frac{d}{dt}PL = -v_3  
\tag{30}
\]

### 9.5 Species PT

**Name** PT  
**Initial concentration** 0 nmol·l⁻¹  
This species takes part in two reactions (as a product in R3 and as a modifier in R5).

\[
\frac{d}{dt}PT = v_3  
\tag{31}
\]
9.6 Species \( \text{Va} \)

**Name** \( \text{Va} \)

**Initial concentration** 0 nmol \( \cdot \) l\(^{-1} \)

This species takes part in two reactions (as a reactant in \( R_3 \) and as a product in \( R_4 \)).

\[
\frac{d}{dt} \text{Va} = v_4 - v_3
\]  

(32)

9.7 Species \( \text{IIa} \)

**Name** \( \text{IIa} \)

**Initial concentration** 0 nmol \( \cdot \) l\(^{-1} \)

This species takes part in five reactions (as a reactant in \( R_7, R_8 \) and as a product in \( R_5, R_6 \) and as a modifier in \( R_4 \)).

\[
\frac{d}{dt} \text{IIa} = v_5 + v_6 - v_7 - v_8
\]  

(33)

9.8 Species \( V \)

**Name** \( V \)

**Initial concentration** 6.711998 nmol \( \cdot \) l\(^{-1} \)

This species takes part in one reaction (as a reactant in \( R_4 \)).

\[
\frac{d}{dt} V = -v_4
\]  

(34)

9.9 Species \( \text{II} \)

**Name** \( \text{II} \)

**Initial concentration** 509.2998 nmol \( \cdot \) l\(^{-1} \)

This species takes part in two reactions (as a reactant in \( R_5, R_6 \)).

\[
\frac{d}{dt} \text{II} = -v_5 - v_6
\]  

(35)

9.10 Species \( \text{IIa}_\text{alpha2M} \)

**Name** \( \text{IIa}_\text{alpha2M} \)

**Initial concentration** 0 nmol \( \cdot \) l\(^{-1} \)

This species takes part in one reaction (as a product in \( R_7 \)).

\[
\frac{d}{dt} \text{IIa}_\text{alpha2M} = v_7
\]  

(36)
9.11 Species IIa_ATIII

Name IIa_ATIII

Initial concentration 0 nmol·l\(^{-1}\)

This species takes part in one reaction (as a product in \(R8\)).

\[
\frac{d}{dt} \text{IIa_ATIII} = v_8 
\]  
(37)

9.12 Species RVV

Name RVV

Initial concentration 0.3349999 nmol·l\(^{-1}\)

This species takes part in one reaction (as a modifier in \(R1\)).

\[
\frac{d}{dt} \text{RVV} = 0 
\]  
(38)

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:0000025 catalytic rate constant: Numerical parameter that quantifies the velocity of an enzymatic reaction

SBO:0000028 enzymatic rate law for irreversible non-modulated non-interacting unireactant enzymes: Kinetics of enzymes that react only with one substance, their substrate. The enzymes do not catalyse the reactions in both directions.

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:0000037 forward trimolecular rate constant, continuous case: Numerical parameter that quantifies the forward velocity of a chemical reaction involving three 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:0000122 mass action rate law for third order forward, first order reverse, reversible reactions, three 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 three 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.

SBO:0000371 Michaelis constant in quasi-steady state situation: Michaelis constant derived using a steady-state assumption for enzyme-substrate and enzyme-product intermediates. For example see Briggs-Haldane equation (SBO:0000031)

SBO:0000461 essential activator: A substance that is absolutely required for occurrence and stimulation of a reaction.