

SBML Model Report

Model identifier: “EnzymaticReaction”



May 17, 2017

1. General Overview

This is a document in SBML Level 2 Version 4 format. Table 1 gives 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	2	Function definitions	0
Parameters	0	Unit definitions	2
Rules	0	Initial assignments	0

2. Unit definitions

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

2.1. Unit definition `per_second`

Definition s^{-1}

2.2. Unit definition `litre_per_mole_per_second`

Definition $\text{mol}^{-1} \cdot \text{l} \cdot \text{s}^{-1}$

2.3. Unit definition `substance`

Name Predefined unit substance

Notes Mole is the predefined SBML unit for substance.

Definition mol

2.4. Unit definition `volume`

Name Predefined unit volume

Notes Litre is the predefined SBML unit for volume.

Definition l

2.5. Unit definition `area`

Name Predefined unit area

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

Definition m^2

2.6. Unit definition `length`

Name Predefined unit length

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

Definition m

2.7. Unit definition `time`

Name Predefined unit time

Notes Second is the predefined SBML unit for time.

Definition s

3. Compartments

This model contains one Compartment.

Table 2: Properties of each Compartment.

ID	Name	SBO	Spatial dimensions	Size	Unit	Constant	Outside
cytosol			3	10^{-14}	l	<input checked="" type="checkbox"/>	

3.1. Compartment `cytosol`

This is an three-dimensional compartment with a constant size of 10^{-14} .

4. Species

This model contains four Species. Section 6 on page 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
ES	ES	cytosol	mol	\varnothing	\varnothing
P	P	cytosol	mol	\varnothing	\varnothing
S	S	cytosol	mol	\varnothing	\varnothing
E	E	cytosol	mol	\varnothing	\varnothing

5. Reactions

This model contains two 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 4: Overview of all Reactions.

Nº	ID	Name	Reaction equation	SBO
1	veq		$E + S \rightleftharpoons ES$	
2	vcat		$ES \longrightarrow E + P$	

5.1. Reaction `veq`

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

Reaction equation



Reactants

Table 5: Properties of each reactant.

Id	Name	SBO
E	E	
S	S	

Products

Table 6: Properties of each product.

Id	Name	SBO
ES	ES	

Kinetic law

Derived unit contains undeclared units

$$v_1 = \text{vol}(\text{cytosol}) \cdot (\text{kon} \cdot [E] \cdot [S] - \text{koff} \cdot [ES]) \quad (2)$$

Table 7: Properties of each Parameter.

ID	Name	SBO	Value	Unit	Constant
kon			1000000.0	$\text{mol}^{-1} \cdot \text{l} \cdot \text{s}^{-1}$	<input checked="" type="checkbox"/>
koff			0.2	s^{-1}	<input checked="" type="checkbox"/>

5.2. Reaction `vcat`

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

Reaction equation



Reactants

Table 8: Properties of each reactant.

Id	Name	SBO
ES	ES	

Products

Table 9: Properties of each product.

Id	Name	SBO
E	E	
P	P	

Kinetic law

Derived unit contains undeclared units

$$v_2 = \text{vol}(\text{cytosol}) \cdot \text{kcat} \cdot [\text{ES}] \quad (4)$$

Table 10: Properties of each Parameter.

ID	Name	SBO	Value	Unit	Constant
kcat			0.1	s ⁻¹	<input checked="" type="checkbox"/>

6. Derived Rate Equations

When interpreted as an ordinary differential equation framework, this model implies the following set of equations for the rate of change of the following 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.

6.1. Species ES

Name ES

Initial amount 0 mol

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

$$\frac{d}{dt}ES = \underbrace{\text{vol}(\text{cytosol}) \cdot (\text{kon} \cdot [E] \cdot [S] - \text{koff} \cdot [ES])}_{v_1} - \underbrace{\text{vol}(\text{cytosol}) \cdot \text{kcat} \cdot [ES]}_{v_2} \quad (5)$$

6.2. Species P

Name P

Initial amount 0 mol

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

$$\frac{d}{dt}P = \underbrace{\text{vol}(\text{cytosol}) \cdot \text{kcat} \cdot [ES]}_{v_2} \quad (6)$$

6.3. Species S

Name S

Initial amount 10^{-20} mol

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

$$\frac{d}{dt}S = - \underbrace{\text{vol}(\text{cytosol}) \cdot (\text{kon} \cdot [E] \cdot [S] - \text{koff} \cdot [ES])}_{v_1} \quad (7)$$

6.4. Species E

Name E

Initial amount $5 \cdot 10^{-21}$ mol

This species takes part in two reactions (as a reactant in [veq](#) and as a product in [vcat](#)).

$$\frac{d}{dt}E = \underbrace{\text{vol}(\text{cytosol}) \cdot k_{\text{cat}} \cdot [\text{ES}]}_{v_2} - \underbrace{\text{vol}(\text{cytosol}) \cdot (k_{\text{on}} \cdot [\text{E}] \cdot [\text{S}] - k_{\text{off}} \cdot [\text{ES}])}_{v_1} \quad (8)$$

A. Document Consistency Report

The given SBML document contains one issue, which is listed in the remainder of this model report. The messages and identification codes shown here are those reported by the [SBML.org online validator](#).

A.1. Error message

This SBML document contains one error message.

Error 0 (SBML Validation Rule #fbc-20209) A `<model>` object must have the required attributes 'strict'. No other attributes from the Flux Balance Constraints namespace are permitted on a `<model>` object. Reference: L3V1 Fbc V2 Section 3.3 Fbc attribute 'strict' is missing from `<Model>` object.