

SBML Model Report

Model name: “Cao2013 - Application of ABSIS in the the enzymatic futile cycle”



May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by the following two authors: Vijayalakshmi Chelliah¹ and Youfang Cao² at September 23rd 2013 at 12:06 a. m. and last time modified at February 24th 2015 at 8:20 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 | 6 |
| events | 0 | constraints | 0 |
| reactions | 6 | function definitions | 0 |
| global parameters | 6 | unit definitions | 0 |
| rules | 0 | initial assignments | 0 |

2 Unit Definitions

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

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2.1 Unit substance

Notes Mole is the predefined SBML unit for substance.

Definition mol

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 m²

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 |
|---------|------|---------|-----------------------|------|-------|-------------------------------------|---------|
| default | | 0000290 | 3 | 1 | litre | <input checked="" type="checkbox"/> | |

3.1 Compartment default

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

SBO:0000290 physical compartment

4 Species

This model contains six 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 Condi- tion |
|----|------|-------------|----------------------------------|-----------|----------------------------|
| S1 | S1 | default | $\text{mol} \cdot \text{l}^{-1}$ | \square | \square |
| S2 | S2 | default | $\text{mol} \cdot \text{l}^{-1}$ | \square | \square |
| S3 | S3 | default | $\text{mol} \cdot \text{l}^{-1}$ | \square | \square |
| S4 | S4 | default | $\text{mol} \cdot \text{l}^{-1}$ | \square | \square |
| S5 | S5 | default | $\text{mol} \cdot \text{l}^{-1}$ | \square | \square |
| S6 | S6 | default | $\text{mol} \cdot \text{l}^{-1}$ | \square | \square |

5 Parameters

This model contains six global parameters.

Table 4: Properties of each parameter.

| Id | Name | SBO | Value | Unit | Constant |
|----|------|-----|-------|------|-------------------------------------|
| k1 | | | 1.0 | | <input checked="" type="checkbox"/> |
| k2 | | | 1.0 | | <input checked="" type="checkbox"/> |
| k3 | | | 0.1 | | <input checked="" type="checkbox"/> |
| k4 | | | 1.0 | | <input checked="" type="checkbox"/> |
| k5 | | | 1.0 | | <input checked="" type="checkbox"/> |
| k6 | | | 0.1 | | <input checked="" type="checkbox"/> |

6 Reactions

This model contains six 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

| Nº | Id | Name | Reaction Equation | SBO |
|----|-----|------|-----------------------------------|-----|
| 1 | re1 | | $S1 + S2 \xrightarrow{S1, S2} S3$ | |
| 2 | re2 | | $S3 \xrightarrow{S3} S1 + S2$ | |
| 3 | re3 | | $S3 \xrightarrow{S3} S1 + S5$ | |
| 4 | re4 | | $S4 + S5 \xrightarrow{S4, S5} S6$ | |
| 5 | re5 | | $S6 \xrightarrow{S6} S4 + S5$ | |
| 6 | re6 | | $S6 \xrightarrow{S6} S4 + S2$ | |

6.1 Reaction `re1`

This is an irreversible reaction of two reactants forming one product influenced by two modifiers.

Reaction equation



Reactants

Table 6: Properties of each reactant.

| Id | Name | SBO |
|----|------|-----|
| S1 | S1 | |
| S2 | S2 | |

Modifiers

Table 7: Properties of each modifier.

| Id | Name | SBO |
|----|------|-----|
| S1 | S1 | |
| S2 | S2 | |

Product

Table 8: Properties of each product.

| Id | Name | SBO |
|----|------|-----|
| S3 | S3 | |

Kinetic Law

Derived unit contains undeclared units

$$v_1 = k_1 \cdot [S1] \cdot [S2] \quad (2)$$

6.2 Reaction `re2`

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

Reaction equation



Reactant

Table 9: Properties of each reactant.

| Id | Name | SBO |
|----|------|-----|
| S3 | S3 | |

Modifier

Table 10: Properties of each modifier.

| Id | Name | SBO |
|----|------|-----|
| S3 | S3 | |

Products

Table 11: Properties of each product.

| Id | Name | SBO |
|----|------|-----|
| S1 | S1 | |
| S2 | S2 | |

Kinetic Law

Derived unit contains undeclared units

$$v_2 = k_2 \cdot [S3] \quad (4)$$

6.3 Reaction re3

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

Reaction equation



Reactant

Table 12: Properties of each reactant.

| Id | Name | SBO |
|----|------|-----|
| S3 | S3 | |

Modifier

Table 13: Properties of each modifier.

| Id | Name | SBO |
|----|------|-----|
| S3 | S3 | |

Products

Table 14: Properties of each product.

| Id | Name | SBO |
|----|------|-----|
| S1 | S1 | |
| S5 | S5 | |

Kinetic Law

Derived unit contains undeclared units

$$v_3 = k_3 \cdot [S3] \quad (6)$$

6.4 Reaction re4

This is an irreversible reaction of two reactants forming one product influenced by two modifiers.

Reaction equation



Reactants

Table 15: Properties of each reactant.

| Id | Name | SBO |
|----|------|-----|
| S4 | S4 | |
| S5 | S5 | |

Modifiers

Table 16: Properties of each modifier.

| Id | Name | SBO |
|----|------|-----|
| S4 | S4 | |
| S5 | S5 | |

Product

Table 17: Properties of each product.

| Id | Name | SBO |
|----|------|-----|
| S6 | S6 | |

Kinetic Law

Derived unit contains undeclared units

$$v_4 = k_4 \cdot [S4] \cdot [S5] \quad (8)$$

6.5 Reaction re5

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

Reaction equation



Reactant

Table 18: Properties of each reactant.

| Id | Name | SBO |
|----|------|-----|
| S6 | S6 | |

Modifier

Table 19: Properties of each modifier.

| Id | Name | SBO |
|----|------|-----|
| S6 | S6 | |

Products

Table 20: Properties of each product.

| Id | Name | SBO |
|----|------|-----|
| S4 | S4 | |
| S5 | S5 | |

Kinetic Law

Derived unit contains undeclared units

$$v_5 = k_5 \cdot [S_6] \quad (10)$$

6.6 Reaction re6

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

Reaction equation



Reactant

Table 21: Properties of each reactant.

| Id | Name | SBO |
|----|------|-----|
| S6 | S6 | |

Modifier

Table 22: Properties of each modifier.

| Id | Name | SBO |
|----|------|-----|
| S6 | S6 | |

Products

Table 23: Properties of each product.

| Id | Name | SBO |
|----|------|-----|
| S4 | S4 | |
| S2 | S2 | |

Kinetic Law

Derived unit contains undeclared units

$$v_6 = k_6 \cdot [S_6] \quad (12)$$

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 S1

Name S1

SBO:0000014 enzyme

Initial amount 0 mol

Charge 0

This species takes part in four reactions (as a reactant in [re1](#) and as a product in [re2](#), [re3](#) and as a modifier in [re1](#)).

$$\frac{d}{dt}S1 = v_2 + v_3 - v_1 \quad (13)$$

7.2 Species S2

Name S2

SBO:0000015 substrate

Initial amount 0 mol

Charge 0

This species takes part in four reactions (as a reactant in [re1](#) and as a product in [re2](#), [re6](#) and as a modifier in [re1](#)).

$$\frac{d}{dt}S2 = v_2 + v_6 - v_1 \quad (14)$$

7.3 Species S3

Name S3

SBO:0000296 macromolecular complex

Initial amount 0 mol

Charge 0

This species takes part in five reactions (as a reactant in [re2](#), [re3](#) and as a product in [re1](#) and as a modifier in [re2](#), [re3](#)).

$$\frac{d}{dt}S3 = v_1 - v_2 - v_3 \quad (15)$$

7.4 Species S4

Name S4

SBO:0000014 enzyme

Initial amount 0 mol

Charge 0

This species takes part in four reactions (as a reactant in [re4](#) and as a product in [re5](#), [re6](#) and as a modifier in [re4](#)).

$$\frac{d}{dt}S4 = v_5 + v_6 - v_4 \quad (16)$$

7.5 Species S5

Name S5

SBO:0000015 substrate

Initial amount 0 mol

Charge 0

This species takes part in four reactions (as a reactant in [re4](#) and as a product in [re3](#), [re5](#) and as a modifier in [re4](#)).

$$\frac{d}{dt}S5 = v_3 + v_5 - v_4 \quad (17)$$

7.6 Species S6

Name S6

SBO:0000296 macromolecular complex

Initial amount 0 mol

Charge 0

This species takes part in five reactions (as a reactant in [re5](#), [re6](#) and as a product in [re4](#) and as a modifier in [re5](#), [re6](#)).

$$\frac{d}{dt}S6 = v_4 - v_5 - v_6 \quad (18)$$

A Glossary of Systems Biology Ontology Terms

SBO:0000014 enzyme: A protein that catalyzes a chemical reaction. The word comes from en “a” or “i”) and simo “leave” or “yeas”)

SBO:0000015 substrate: Molecule which is acted upon by an enzyme. The substrate binds with the enzyme’s active site, and the enzyme catalyzes a chemical reaction involving the substrate

SBO:0000290 physical compartment: Specific location of space, that can be bounded or not. A physical compartment can have 1, 2 or 3 dimensions

SBO:0000296 macromolecular complex: Non-covalent complex of one or more macromolecules and zero or more simple chemicals

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