SBML Model Report

Model name: "Ferreira2003_CML_generation2"

May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 3 format. This model was created by Harish Dharuri[1] at April nineth 2006 at 8:54 p. m. and last time modified at October nineth 2014 at 3:39 p. m. Table 1 shows 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	12	function definitions	0
global parameters	2	unit definitions	1
rules	2	initial assignments	0

Model Notes

The model should reproduce the figure 2F of the article.

The equation 7 has been split into equations 7a-7c, in order to take into account the different flux rates of Lysine and CML formation from Schiff.

The model was tested in Jarnac (SBML L2 V1) and Copasi (SBML L2 V3).

[1] California Institute of Technology, hdharuri@cds.caltech.edu

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2 Unit Definitions

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

2.1 Unit `time`

Name hour (default)

Definition 3600 s

2.2 Unit `substance`

Notes Mole is the predefined SBML unit for `substance`.

Definition mol

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`			3	1	litre	☑	

3.1 Compartment `compartment`

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

4 Species

This model contains six species. Section 8 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
Glucose		compartment	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Lysine		compartment	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Schiff		compartment	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Amadori		compartment	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Glyoxal		compartment	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
CML		compartment	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟

5 Parameters

This model contains two global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Fraction_Amadori			0.0		⊟
Fraction_CML			0.0		⊟

6 Rules

This is an overview of two rules.

6.1 Rule Fraction_Amadori

Rule Fraction_Amadori is an assignment rule for parameter Fraction_Amadori:

$$\text{Fraction\_Amadori} = \frac{[\text{Amadori}]}{0.0034} \tag{1}$$

6.2 Rule Fraction_CML

Rule Fraction_CML is an assignment rule for parameter Fraction_CML:

$$\text{Fraction\_CML} = \frac{[\text{CML}]}{0.0034} \tag{2}$$

7 Reactions

This model contains twelve 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	v1a		$\text{Lysine} + \text{Glucose} \longrightarrow \text{Schiff}$	
2	v1b		$\text{Schiff} \longrightarrow \text{Lysine} + \text{Glucose}$	
3	v2a		$\text{Schiff} \longrightarrow \text{Amadori}$	
4	v2b		$\text{Amadori} \longrightarrow \text{Schiff}$	
5	v3		$\text{Glucose} \longrightarrow \text{Glyoxal}$	
6	v4		$\text{Amadori} \longrightarrow \text{CML}$	
7	v5		$\text{Lysine} + \text{Glyoxal} \longrightarrow \text{CML}$	
8	v5b		$\text{Glyoxal} \longrightarrow \emptyset$	
9	v6		$\text{Schiff} \longrightarrow \text{CML}$	
10	v7a		$\emptyset \xrightarrow{\text{Schiff}} \text{Lysine}$	
11	v7b		$\emptyset \xrightarrow{\text{Schiff}} \text{Glyoxal}$	
12	v7c		$\text{Schiff} \longrightarrow \emptyset$	

7.1 Reaction v1a

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

Reaction equation

$$\text{Lysine} + \text{Glucose} \longrightarrow \text{Schiff} \tag{3}$$

Reactants

Table 6: Properties of each reactant.

Id	Name	SBO
Lysine		
Glucose		

Product

Table 7: Properties of each product.

Id	Name	SBO
Schiff		

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \text{vol}(\text{compartment}) \cdot \text{p1} \cdot \text{k1a} \cdot [\text{Glucose}] \cdot [\text{Lysine}] \tag{4}$$

Table 8: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
p1			0.115		☑
k1a			0.090		☑

7.2 Reaction v1b

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

Reaction equation

$$\text{Schiff} \longrightarrow \text{Lysine} + \text{Glucose} \tag{5}$$

Reactant

Table 9: Properties of each reactant.

Id	Name	SBO
Schiff		

Products

Table 10: Properties of each product.

Id	Name	SBO
Lysine		
Glucose		

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \text{vol}\,(\text{compartment}) \cdot \text{k1b} \cdot [\text{Schiff}] \tag{6}$$

Table 11: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1b			0.36		☑

7.3 Reaction v2a

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

Reaction equation

$$\text{Schiff} \longrightarrow \text{Amadori} \tag{7}$$

Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
Schiff		

Product

Table 13: Properties of each product.

Id	Name	SBO
Amadori		

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{p2} \cdot \mathrm{k2a} \cdot [\mathrm{Schiff}] \tag{8}$$

Table 14: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
p2			0.750		☑
k2a			0.033		☑

7.4 Reaction v2b

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

Reaction equation

$$\mathrm{Amadori} \longrightarrow \mathrm{Schiff} \tag{9}$$

Reactant

Table 15: Properties of each reactant.

Id	Name	SBO
Amadori		

Product

Table 16: Properties of each product.

Id	Name	SBO
Schiff		

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{p2} \cdot \mathrm{k2b} \cdot [\mathrm{Amadori}] \tag{10}$$

Table 17: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
p2			0.750		☑
k2b			0.001		☑

7.5 Reaction v3

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

Reaction equation

$$\mathrm{Glucose} \longrightarrow \mathrm{Glyoxal} \tag{11}$$

Reactant

Table 18: Properties of each reactant.

Id	Name	SBO
Glucose		

Product

Table 19: Properties of each product.

Id	Name	SBO
Glyoxal		

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{ox} \cdot \mathrm{p3} \cdot \mathrm{k3} \cdot \left(\frac{[\mathrm{Glucose}]}{0.25}\right)^{0.36} \tag{12}$$

Table 20: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
ox			1.000		☑
p3			1.000		☑
k3			$7.92 \cdot 10^{-7}$		☑

7.6 Reaction v4

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

Reaction equation

$$\mathrm{Amadori} \longrightarrow \mathrm{CML} \tag{13}$$

Reactant

Table 21: Properties of each reactant.

Id	Name	SBO
Amadori		

Product

Table 22: Properties of each product.

Id	Name	SBO
CML		

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{ox} \cdot \mathrm{p4} \cdot \mathrm{k4} \cdot [\mathrm{Amadori}] \tag{14}$$

Table 23: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
ox			1.000		☑
p4			1.000		☑
k4			$8.6 \cdot 10^{-5}$		☑

7.7 Reaction v5

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

Reaction equation

$$\text{Lysine} + \text{Glyoxal} \longrightarrow \text{CML} \tag{15}$$

Reactants

Table 24: Properties of each reactant.

Id	Name	SBO
Lysine		
Glyoxal		

Product

Table 25: Properties of each product.

Id	Name	SBO
CML		

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \text{vol}\,(\text{compartment}) \cdot \text{ox} \cdot \text{p5} \cdot \text{k5} \cdot [\text{Glyoxal}] \cdot [\text{Lysine}] \tag{16}$$

Table 26: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
ox			1.000		☑
p5			1.000		☑
k5			0.019		☑

7.8 Reaction v5b

This is an irreversible reaction of one reactant forming no product.

Reaction equation

$$\text{Glyoxal} \longrightarrow \emptyset \tag{17}$$

Reactant

Table 27: Properties of each reactant.

Id	Name	SBO
Glyoxal		

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \text{vol}\,(\text{compartment}) \cdot \text{k5b} \cdot [\text{Glyoxal}] \tag{18}$$

Table 28: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k5b			0.002		☑

7.9 Reaction v6

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

Reaction equation

$$\text{Schiff} \longrightarrow \text{CML} \tag{19}$$

Reactant

Table 29: Properties of each reactant.

Id	Name	SBO
Schiff		

Product

Table 30: Properties of each product.

Id	Name	SBO
CML		

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{ox} \cdot \mathrm{p6} \cdot \mathrm{k3} \cdot \left(\frac{[\mathrm{Schiff}]}{0.25}\right)^{0.36} \tag{20}$$

Table 31: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
ox			1.000		☑
p6			2.700		☑
k3			$7.92 \cdot 10^{-7}$		☑

7.10 Reaction v7a

This is an irreversible reaction of no reactant forming one product influenced by one modifier.

Reaction equation

$$\emptyset \xrightarrow{\text{Schiff}} \text{Lysine} \tag{21}$$

Modifier

Table 32: Properties of each modifier.

Id	Name	SBO
Schiff		

Product

Table 33: Properties of each product.

Id	Name	SBO
Lysine		

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = \mathrm{vol}\,(\mathrm{compartment}) \cdot 0.05 \cdot \mathrm{ox} \cdot \mathrm{p7} \cdot \mathrm{k3} \cdot \left(\frac{[\mathrm{Schiff}]}{0.25}\right)^{0.36} \tag{22}$$

Table 34: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
ox			1.000		☑
p7			60.000		☑
k3			$7.92 \cdot 10^{-7}$		☑

7.11 Reaction v7b

This is an irreversible reaction of no reactant forming one product influenced by one modifier.

Reaction equation

$$\emptyset \xrightarrow{\mathrm{Schiff}} \mathrm{Glyoxal} \tag{23}$$

Modifier

Table 35: Properties of each modifier.

Id	Name	SBO
Schiff		

Product

Table 36: Properties of each product.

Id	Name	SBO
Glyoxal		

Kinetic Law

Derived unit contains undeclared units

$$v_{11} = \mathrm{vol}\,(\mathrm{compartment}) \cdot 0.0050 \cdot \mathrm{ox} \cdot \mathrm{p7} \cdot \mathrm{k3} \cdot \left(\frac{[\mathrm{Schiff}]}{0.25}\right)^{0.36} \tag{24}$$

Table 37: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
ox			1.000		☑
p7			60.000		☑
k3			$7.92 \cdot 10^{-7}$		☑

7.12 Reaction v7c

This is an irreversible reaction of one reactant forming no product.

Reaction equation

$$\mathrm{Schiff} \longrightarrow \emptyset \tag{25}$$

Reactant

Table 38: Properties of each reactant.

Id	Name	SBO
Schiff		

Kinetic Law

Derived unit contains undeclared units

$$v_{12} = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{ox} \cdot \mathrm{p7} \cdot \mathrm{k3} \cdot \left(\frac{[\mathrm{Schiff}]}{0.25}\right)^{0.36} \tag{26}$$

Table 39: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
ox			1.000		☑
p7			60.000		☑

Id	Name	SBO	Value	Unit	Constant
k3			$7.92 \cdot 10^{-7}$		☑

8 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.

8.1 Species `Glucose`

Initial concentration $0.25\ \mathrm{mol} \cdot \mathrm{l}^{-1}$

This species takes part in three reactions (as a reactant in `v1a`, `v3` and as a product in `v1b`).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Glucose} = v_2 - v_1 - v_5 \tag{27}$$

8.2 Species `Lysine`

Initial concentration $0.0034\ \mathrm{mol} \cdot \mathrm{l}^{-1}$

This species takes part in four reactions (as a reactant in `v1a`, `v5` and as a product in `v1b`, `v7a`).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Lysine} = v_2 + v_{10} - v_1 - v_7 \tag{28}$$

8.3 Species `Schiff`

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

This species takes part in eight reactions (as a reactant in `v1b`, `v2a`, `v6`, `v7c` and as a product in `v1a`, `v2b` and as a modifier in `v7a`, `v7b`).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Schiff} = v_1 + v_4 - v_2 - v_3 - v_9 - v_{12} \tag{29}$$

8.4 Species Amadori

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

This species takes part in three reactions (as a reactant in v2b, v4 and as a product in v2a).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Amadori} = v_3 - v_4 - v_6 \tag{30}$$

8.5 Species Glyoxal

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

This species takes part in four reactions (as a reactant in v5, v5b and as a product in v3, v7b).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Glyoxal} = v_5 + v_{11} - v_7 - v_8 \tag{31}$$

8.6 Species CML

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

This species takes part in three reactions (as a product in v4, v5, v6).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{CML} = v_6 + v_7 + v_9 \tag{32}$$

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