SBML Model Report

Model identifier: "Nutrient_transition_counter"



July 19, 2016

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	14
events	0	constraints	0
reactions	12	function definitions	0
global parameters	0	unit definitions	5
rules	0	initial assignments	0

2. Unit Definitions

This is an overview of five unit definitions.

2.1. Unit substance

Name substance

Definition mol

2.2. Unit volume

Name volume

Definition 1

2.3. Unit area

Name area

Definition m²

2.4. Unit length

Name length

Definition m

2.5. Unit time

Name 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			3	1	litre	Ø	

3.1. Compartment default

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

4. Species

This model contains 14 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 Condi- tion
Gal	Gal	default	invalid		
Glu	Glu	default	invalid		
${\tt Gal_Sensor}$	Gal Sensor	default	invalid		
Degraded_Glu	Degraded_Glu	default	invalid		
Degraded_Gal	Degraded_Gal	default	invalid		
${\tt Glu_Sensor}$	Glu Sensor	default	invalid		
${\tt Gal_Activator}$	Gal Activator	default	invalid		
${\tt Glu_to_Gal}$	Glu-to-Gal	default	invalid		
${ t Glu_Activator}$	Glu Activator	default	invalid		
${\tt Gal_to_Glu}$	Gal-to-Glu	default	invalid		
Degraded_Glu- _Sensor	Degraded_Glu_Sensor	default	invalid		
Degraded_Gal- _Sensor	Degraded_Gal_Sensor	default	invalid		
Degraded_Glu_To- _Gal	Degraded_Glu_To_Gal	default	invalid		
Degraded_Gal_To- _Glu	Degraded_Gal_To_Glu	default	invalid		

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5. 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 one or more modifiers, the identifiers of the modifier species are written above the reaction arrow.

Table 4: Overview of all reactions

$N_{\bar{0}}$	Id	Name	Reaction Equation SBO
1	re1	re1	extstyle ext
2	re8	re8	extstyle ext
3	re3	re3	${ t Glu_Sensor} \longrightarrow { t Degraded_Glu_Sensor}$
4	re12	re12	${\tt Gal} \longrightarrow {\tt Glu_Sensor} + {\tt Gal}$
5	re2	re2	${ t Gal_Sensor} \longrightarrow { t Degraded_Gal_Sensor}$
6	re6	re6	${ t Gal_Sensor} + { t Gal} \Longrightarrow { t Gal_Activator}$
7	re4	re4	$\texttt{Glu} \longrightarrow \texttt{Gal_Sensor} + \texttt{Glu}$
8	re5	re5	${ t Gal_Activator} \hspace{0.5cm} \longrightarrow \hspace{0.5cm} { t Glu_to_Gal} \hspace{0.5cm} + \hspace{0.5cm}$
			Gal_Activator
9	re7	re7	${ t Glu_to_Gal} \longrightarrow { t Degraded_Glu_To_Gal}$
10	re11	re11	${ t Gal_to_Glu} \longrightarrow { t Degraded_Gal_To_Glu}$
11	re9	re9	${ t Glu_Activator} \hspace{0.5cm} \longrightarrow \hspace{0.5cm} { t Gal_to_Glu} \hspace{0.5cm} + \hspace{0.5cm}$
			${ t Glu_Activator}$
12	re10	re10	${ t Glu_Sensor} + { t Glu} \Longrightarrow { t Glu_Activator}$

5.1. Reaction re1

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

Name re1

Reaction equation

$$Glu \longrightarrow Degraded_Glu$$
 (1)

Reactant

Table 5: Properties of each reactant.

Id	Name	SBO
Glu	Glu	

Product

Table 6: Properties of each product.

Id	Name	SBO
Degraded_Glu	Degraded_Glu	

Kinetic Law

Derived unit not available

$$v_1 = Glu \cdot glu_deg_k$$
 (2)

Table 7: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
glu_deg_k	glu_deg_k	10.0 mol	$ \checkmark $

5.2. Reaction re8

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

Name re8

Reaction equation

$$Gal \longrightarrow Degraded_Gal$$
 (3)

Reactant

Table 8: Properties of each reactant.

Id	Name	SBO
Gal	Gal	

Product

Table 9: Properties of each product.

Id	Name	SBO
Degraded_Gal	Degraded_Gal	

Kinetic Law

Derived unit not available

$$v_2 = [Gal] \cdot gal_deg_k \tag{4}$$

Table 10: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
gal_deg_k	gal_deg_k	10.0 mol	

5.3. Reaction re3

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

Name re3

Reaction equation

$$Glu_Sensor \longrightarrow Degraded_Glu_Sensor$$
 (5)

Reactant

Table 11: Properties of each reactant.

Id	Name	SBO
Glu_Sensor	Glu Sensor	

Product

Table 12: Properties of each product.

Id	Name	SBO
Degraded_Glu_Sensor	Degraded_Glu_Sensor	

Kinetic Law

Derived unit not available

$$v_3 = [Glu_Sensor] \cdot glu_sensor_deg_k$$
 (6)

Table 13: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
glu_sensor- _deg_k	glu_sensor_deg_k		1.0	mol	✓

5.4. Reaction re12

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

Name re12

Reaction equation

$$Gal \longrightarrow Glu_Sensor + Gal$$
 (7)

Reactant

Table 14: Properties of each reactant.

Id	Name	SBO
Gal	Gal	

Products

Table 15: Properties of each product.

Id	Name	SBO
Glu_Sensor		
Gal	Gal	

Kinetic Law

Derived unit not available

$$v_4 = [Gal] \cdot k1 \tag{8}$$

Table 16: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	k1	1.0 mol	

5.5. Reaction re2

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

Name re2

Reaction equation

$$\texttt{Gal_Sensor} \longrightarrow \texttt{Degraded_Gal_Sensor} \tag{9}$$

Reactant

Table 17: Properties of each reactant.

Id	Name	SBO
Gal_Sensor	Gal Sensor	

Product

Table 18: Properties of each product.

	F	
Id	Name	SBO
-		
Degraded_Gal_Sensor	Degraded_Gal_Sensor	

Kinetic Law

Derived unit not available

$$v_5 = [Gal_Sensor] \cdot gal_sensor_deg_k$$
 (10)

Table 19: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
gal_sensor- _deg_k	gal_sensor_deg_k		1.0	mol	Ø

5.6. Reaction re6

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

Name re6

Reaction equation

$$Gal_Sensor + Gal \rightleftharpoons Gal_Activator$$
 (11)

Reactants

Table 20: Properties of each reactant.

Id	Name	SBO
${\tt Gal_Sensor}$	Gal Sensor	
Gal	Gal	

Product

Table 21: Properties of each product.

Id	Name	SBO
Gal Activator	Gal Activator	

Id	Name	SBO

Kinetic Law

Derived unit contains undeclared units

$$v_6 = [Gal_Sensor] \cdot [Gal] \cdot gal_act_kf - gal_act_kr \cdot [Gal_Activator]$$
 (12)

Table 22: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
gal_act_kf	gal_act_kf	1.0 mol	lacksquare
gal_act_kr	gal_act_kr	1.0 mol	

5.7. Reaction re4

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

Name re4

Reaction equation

$$Glu \longrightarrow Gal_Sensor + Glu$$
 (13)

Reactant

Table 23: Properties of each reactant.

Id	Name	SBO
Glu	Glu	

Products

Table 24: Properties of each product.

Id	Name	SBO
Gal_Sensor Glu	Gal Sensor Glu	

Kinetic Law

Derived unit not available

$$v_7 = Glu \cdot k1 \tag{14}$$

Table 25: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	k1	1.0 mol	

5.8. Reaction re5

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

Name re5

Reaction equation

$$Gal_Activator \longrightarrow Glu_to_Gal + Gal_Activator$$
 (15)

Reactant

Table 26: Properties of each reactant.

Id	Name	SBO
Gal_Activator	Gal Activator	

Products

Table 27: Properties of each product.

Id	Name	SBO
Glu_to_Gal Gal_Activator	Glu-to-Gal Gal Activator	

Kinetic Law

Derived unit not available

$$v_8 = [Gal_Activator] \cdot k2$$
 (16)

Table 28: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
glu_to_gal_k	glu_to_gal_k		1.0	mol	
k2	k2		1.0	mol	

5.9. Reaction re7

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

Name re7

Reaction equation

$$\texttt{Glu_to_Gal} \longrightarrow \texttt{Degraded_Glu_To_Gal} \tag{17}$$

Reactant

Table 29: Properties of each reactant.

Id	Name	SBO
Glu_to_Gal	Glu-to-Gal	

Product

Table 30: Properties of each product.

Id	Name	SBO
Degraded_Glu_To_Gal	Degraded_Glu_To_Gal	

Kinetic Law

Derived unit not available

$$v_9 = [Glu_to_Gal] \cdot glu_to_gal_deg_k$$
 (18)

Table 31: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
glu_to_gal- _deg_k	glu_to_gal_deg_k		0.001	mol	

5.10. Reaction re11

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

Name re11

Reaction equation

$$Gal_to_Glu \longrightarrow Degraded_Gal_To_Glu$$
 (19)

Reactant

Table 32: Properties of each reactant.

Id	Name	SBO
Gal_to_Glu	Gal-to-Glu	-

Product

Table 33: Properties of each product.

Id	Name	SBO
Degraded_Gal_To_Glu	Degraded_Gal_To_Glu	

Kinetic Law

Derived unit not available

$$v_{10} = [Gal_to_Glu] \cdot gal_to_glu_deg_k$$
 (20)

Table 34: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
gal_to_glu- _deg_k	gal_to_glu_deg_k		0.001	mol	

5.11. Reaction re9

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

Name re9

Reaction equation

$$Glu_Activator \longrightarrow Gal_to_Glu+Glu_Activator$$
 (21)

Reactant

Table 35: Properties of each reactant.

Id	Name	SBO
Glu_Activator	Glu Activator	

Products

Table 36: Properties of each product.

Id	Name	SBO
Gal_to_Glu Glu_Activator	Gal-to-Glu Glu Activator	

Kinetic Law

Derived unit not available

$$v_{11} = [Glu_Activator] \cdot k1$$
 (22)

Table 37: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
gal_to_glu_k k1	gal_to_glu_k k1		1.0 1.0	mol mol	✓

5.12. Reaction re10

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

Name re10

Reaction equation

$$Glu_Sensor + Glu \Longrightarrow Glu_Activator$$
 (23)

Reactants

Table 38: Properties of each reactant.

Id	Name	SBO
Glu_Sensor Glu	Glu Sensor Glu	

Product

Table 39: Properties of each product.

Id	Name	SBO
Glu_Activator	Glu Activator	

Kinetic Law

Derived unit contains undeclared units

$$v_{12} = [Glu_Sensor] \cdot Glu \cdot glu_act_kf - glu_act_kr \cdot [Glu_Activator]$$
 (24)

Table 40: Properties of each parameter.

Id	Name	SBO Valu	e Unit	Constant
glu_act_kf	glu_act_kf	1.0	mol	
${ t glu_act_kr}$	glu_act_kr	1.0	mol	

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 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 Gal

Name Gal

Initial amount 0 mol

This species takes part in four reactions (as a reactant in re8, re12, re6 and as a product in re12).

$$\frac{d}{dt}Gal = |v_4| - |v_2| - |v_4| - |v_6| \tag{25}$$

6.2. Species Glu

Name Glu

Initial amount 0 mol

Charge 0

This species takes part in four reactions (as a reactant in re1, re4, re10 and as a product in re4).

$$\frac{d}{dt}Glu = |v_7| - |v_1| - |v_7| - |v_{12}|$$
 (26)

6.3. Species Gal_Sensor

Name Gal Sensor

Initial amount 0 mol

This species takes part in three reactions (as a reactant in re2, re6 and as a product in re4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Gal_Sensor} = |v_7| - |v_5| - |v_6| \tag{27}$$

6.4. Species Degraded_Glu

Name Degraded_Glu

Initial amount 0 mol

This species takes part in one reaction (as a product in re1).

$$\frac{\mathrm{d}}{\mathrm{d}t} \mathrm{Degraded_Glu} = |v_1| \tag{28}$$

6.5. Species Degraded_Gal

Name Degraded_Gal

Initial amount 0 mol

This species takes part in one reaction (as a product in re8).

$$\frac{\mathrm{d}}{\mathrm{d}t} \mathsf{Degraded_Gal} = v_2 \tag{29}$$

6.6. Species Glu_Sensor

Name Glu Sensor

Initial amount 0 mol

This species takes part in three reactions (as a reactant in re3, re10 and as a product in re12).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Glu.Sensor} = v_4 - v_3 - v_{12} \tag{30}$$

6.7. Species Gal_Activator

Name Gal Activator

Initial amount 0 mol

This species takes part in three reactions (as a reactant in re5 and as a product in re6, re5).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Gal}_{-}\mathrm{Activator} = |v_6| + |v_8| - |v_8| \tag{31}$$

6.8. Species Glu_to_Gal

Name Glu-to-Gal

Initial amount 0 mol

This species takes part in two reactions (as a reactant in re7 and as a product in re5).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Glu_to_Gal} = |v_8| - |v_9| \tag{32}$$

6.9. Species Glu_Activator

Name Glu Activator

Initial amount 0 mol

This species takes part in three reactions (as a reactant in re9 and as a product in re9, re10).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Glu_Activator} = |v_{11}| + |v_{12}| - |v_{11}| \tag{33}$$

6.10. Species Gal_to_Glu

Name Gal-to-Glu

Initial amount 0 mol

This species takes part in two reactions (as a reactant in rel1 and as a product in re9).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Gal_to_Glu} = v_{11} - v_{10} \tag{34}$$

6.11. Species Degraded_Glu_Sensor

Name Degraded_Glu_Sensor

Initial amount 0 mol

This species takes part in one reaction (as a product in re3).

$$\frac{\mathrm{d}}{\mathrm{d}t} \mathsf{Degraded_Glu_Sensor} = v_3 \tag{35}$$

6.12. Species Degraded_Gal_Sensor

Name Degraded_Gal_Sensor

Initial amount 0 mol

This species takes part in one reaction (as a product in re2).

$$\frac{\mathrm{d}}{\mathrm{d}t} \text{Degraded_Gal_Sensor} = v_5 \tag{36}$$

6.13. Species Degraded_Glu_To_Gal

Name Degraded_Glu_To_Gal

Initial amount 0 mol

This species takes part in one reaction (as a product in re7).

$$\frac{\mathrm{d}}{\mathrm{d}t} \mathsf{Degraded_Glu_To_Gal} = v_9 \tag{37}$$

6.14. Species Degraded_Gal_To_Glu

Name Degraded_Gal_To_Glu

Initial amount 0 mol

This species takes part in one reaction (as a product in re11).

$$\frac{\mathrm{d}}{\mathrm{d}t} \mathsf{Degraded_Gal_To_Glu} = v_{10} \tag{38}$$

A. Model Consistency Report

Currently, the JavaTM library JSBML, which is used by the documentation tool SBML ATEX, does not provide an implementation for full SBML consistency checks. Hence, at this position this report cannot highlight any problems in the SBML document, which does not mean that it is entirely correct. Please visit the website sbml.org and use the SBML validator there.

References

Dräger, A., Planatscher, H., Wouamba, D. M., Schröder, A., Hucka, M., Endler, L., Golebiewski, M., Müller, W., and Zell, A. (2009). SBML2IATEX: Conversion of SBML files into human-readable reports. Bioinformatics, **25**(11), 1455–1456. 10.1093/bioinformatics/btp170.