SBML Model Report

Model name: "Smallbone2011_TrehaloseBiosynthesis"

May 5, 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 Chelliah[1] and Kieran Smallbone[2] at July twelveth 2010 at no o' clock in the morning. and last time modified at May 16th 2012 at 2:48 p. m. Table 1 gives 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	2
species types	0	species	16
events	0	constraints	0
reactions	8	function definitions	0
global parameters	13	unit definitions	5
rules	6	initial assignments	6

Model Notes

This model is from the article:
Building a Kinetic Model of Trehalose Biosynthesis in Saccharomyces cerevisiae.
Smallbone K, Malys N, Messiha HL, Wishart JA, Simeonidis E. Methods Enzymol. 2011;500:355-70. 21943906 ,

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Abstract:
In this chapter, we describe the steps needed to create a kinetic model of a metabolic pathway based on kinetic data from experimental measurements and literature review. Our methodology is presented by utilizing the example of trehalose metabolism in yeast. The biology of the trehalose cycle is briefly reviewed and discussed.

2 Unit Definitions

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

2.1 Unit `substance`

Name mmol

Definition mmol

2.2 Unit `time`

Name min

Definition 60 s

2.3 Unit `mM`

Name mM

Definition $\mathrm{mmol} \cdot \mathrm{l}^{-1}$

2.4 Unit `per_min`

Name per min

Definition $(60\ \mathrm{s})^{-1}$

2.5 Unit mM_per_min

Name mM per min

Definition $\mathrm{mmol} \cdot \mathrm{l}^{-1} \cdot (60\ \mathrm{s})^{-1}$

2.6 Unit volume

Notes Litre is the predefined SBML unit for `volume`.

Definition l

2.7 Unit area

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

Definition m^2

2.8 Unit length

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

Definition m

3 Compartments

This model contains two compartments.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
`cell`	cell		3	1	litre	☑	`medium`
`medium`	medium		3	1	litre	☑	

3.1 Compartment cell

This is a three dimensional compartment with a constant size of one litre, which is surrounded by `medium` (medium).

Name cell

3.2 Compartment medium

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

Name medium

4 Species

This model contains 16 species. The boundary condition of ten of these species is set to `true` so that these species' amount cannot be changed by any reaction. Section 9 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
`glc`	glucose	`cell`	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
`g1p`	glucose 1-phosphate	`cell`	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
`g6p`	glucose 6-phosphate	`cell`	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
`trh`	trehalose	`cell`	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
`t6p`	trehalose 6-phosphate	`cell`	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
`udg`	UDP glucose	`cell`	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
`adp`	ADP	`cell`	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	☑
`atp`	ATP	`cell`	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	☑
`ppi`	diphosphate	`cell`	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	☑
`f6p`	fructose 6-phosphate	`cell`	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	☑
`h`	H+	`cell`	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	☑
`pho`	phosphate	`cell`	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	☑
`udp`	UDP	`cell`	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	☑
`utp`	UTP	`cell`	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	☑
`h2o`	water	`cell`	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	☑
`glx`	glucose	`medium`	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	☑

5 Parameters

This model contains 13 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
heat	heat		0.000	dimensionless	☑
glc_0			0.098	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
glc_change	log10 change in glucose		0.000	dimensionless	☐
g1p_0			0.100	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
g1p_change	log10 change in glucose 1-phosphate		0.000	dimensionless	☐
g6p_0			2.675	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
g6p_change	log10 change in glucose 6-phosphate		0.000	dimensionless	☐
trh_0			0.050	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
trh_change	log10 change in trehalose		0.000	dimensionless	☐
t6p_0			0.020	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
t6p_change	log10 change in trehalose 6-phosphate		0.000	dimensionless	☐
udg_0			0.700	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
udg_change	log10 change in UDP glucose		0.000	dimensionless	☐

6 Initialassignments

This is an overview of six initialassignments.

6.1 Initialassignment glc

Derived unit $\mathrm{mmol} \cdot \mathrm{l}^{-1}$

Math glc_0

6.2 Initialassignment g1p

Derived unit $\mathrm{mmol} \cdot \mathrm{l}^{-1}$

Math g1p_0

6.3 Initialassignment g6p

Derived unit $\mathrm{mmol} \cdot \mathrm{l}^{-1}$

Math g6p_0

6.4 Initialassignment trh

Derived unit $\mathrm{mmol} \cdot \mathrm{l}^{-1}$

Math trh_0

6.5 Initialassignment t6p

Derived unit $\mathrm{mmol} \cdot \mathrm{l}^{-1}$

Math t6p_0

6.6 Initialassignment udg

Derived unit $\mathrm{mmol} \cdot \mathrm{l}^{-1}$

Math udg_0

7 Rules

This is an overview of six rules.

7.1 Rule glc_change

Rule glc_change is an assignment rule for parameter glc_change:

$$\mathrm{glc\_change} = \log_{10}\left(\frac{[\mathrm{glc}]}{\mathrm{glc\_0}}\right) \tag{1}$$

Derived unit dimensionless

7.2 Rule g1p_change

Rule g1p_change is an assignment rule for parameter g1p_change:

$$\mathrm{g1p\_change} = \log_{10}\left(\frac{[\mathrm{g1p}]}{\mathrm{g1p\_0}}\right) \tag{2}$$

Derived unit dimensionless

7.3 Rule g6p_change

Rule g6p_change is an assignment rule for parameter g6p_change:

$$\text{g6p\_change} = \log_{10}\left(\frac{[\text{g6p}]}{\text{g6p\_0}}\right) \tag{3}$$

Derived unit dimensionless

7.4 Rule trh_change

Rule trh_change is an assignment rule for parameter trh_change:

$$\text{trh\_change} = \log_{10}\left(\frac{[\text{trh}]}{\text{trh\_0}}\right) \tag{4}$$

Derived unit dimensionless

7.5 Rule t6p_change

Rule t6p_change is an assignment rule for parameter t6p_change:

$$\text{t6p\_change} = \log_{10}\left(\frac{[\text{t6p}]}{\text{t6p\_0}}\right) \tag{5}$$

Derived unit dimensionless

7.6 Rule udg_change

Rule udg_change is an assignment rule for parameter udg_change:

$$\text{udg\_change} = \log_{10}\left(\frac{[\text{udg}]}{\text{udg\_0}}\right) \tag{6}$$

Derived unit dimensionless

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

№	Id	Name	Reaction Equation	SBO
1	pgi	G6P isomerase	$g6p \rightleftharpoons f6p$	0000176
2	hxt	glucose transport	$glx \rightleftharpoons glc$	0000185
3	hxk	hexokinase	$glc + atp \xrightarrow{t6p} g6p + adp + h$	0000176
4	pgm	phosphoglucomutase	$g6p \rightleftharpoons g1p$	0000176
5	tpp	T6P phosphatase	$t6p + h2o \longrightarrow trh + pho$	0000176
6	tps	T6P synthase	$g6p + udg \longrightarrow t6p + udp + h$	0000176
7	nth	trehalase	$trh + h2o \longrightarrow 2\,glc$	0000176
8	ugp	UDP glucose phosphorylase	$g1p + utp + h \longrightarrow udg + ppi$	0000176

8.1 Reaction pgi

This is a reversible reaction of one reactant forming one product.

Name G6P isomerase

SBO:0000176 biochemical reaction

Reaction equation

$$\mathrm{g6p} \rightleftharpoons \mathrm{f6p} \tag{7}$$

Reactant

Table 6: Properties of each reactant.

Id	Name	SBO
g6p	glucose 6-phosphate	

Product

Table 7: Properties of each product.

Id	Name	SBO
f6p	fructose 6-phosphate	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \frac{\frac{\mathrm{vol(cell)} \cdot \mathrm{shock}^{\mathrm{heat}} \cdot \mathrm{Vmax}}{\mathrm{Kg6p}} \cdot \left([\mathrm{g6p}] - \frac{[\mathrm{f6p}]}{\mathrm{Keq}} \right)}{1 + \frac{[\mathrm{g6p}]}{\mathrm{Kg6p}} + \frac{[\mathrm{f6p}]}{\mathrm{Kf6p}}} \tag{8}$$

Table 8: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax			1071.00	$\mathrm{mmol} \cdot 1^{-1} \cdot (60\ \mathrm{s})^{-1}$	☑
Kg6p			1.40	$\mathrm{mmol} \cdot 1^{-1}$	☑
Kf6p			0.29	$\mathrm{mmol} \cdot 1^{-1}$	☑
Keq			0.30	dimensionless	☑
shock			1.00	dimensionless	☑

8.2 Reaction hxt

This is a reversible reaction of one reactant forming one product.

Name glucose transport

SBO:0000185 transport reaction

Reaction equation

$$\mathrm{glx} \rightleftharpoons \mathrm{glc} \tag{9}$$

Reactant

Table 9: Properties of each reactant.

Id	Name	SBO
glx	glucose	

Product

Table 10: Properties of each product.

Id	Name	SBO
glc	glucose	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \frac{\frac{\mathrm{vol(cell)} \cdot \mathrm{shock}^{\mathrm{heat}} \cdot \mathrm{Vmax} \cdot ([\mathrm{glx}] - [\mathrm{glc}])}{\mathrm{Kglc}}}{1 + \frac{[\mathrm{glx}] + [\mathrm{glc}]}{\mathrm{Kglc}} + \frac{\mathrm{Ki} \cdot [\mathrm{glx}] \cdot [\mathrm{glc}]}{\mathrm{Kglc}^2}} \tag{10}$$

Table 11: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax			97.240	$\mathrm{mmol} \cdot \mathrm{l}^{-1} \cdot (60\ \mathrm{s})^{-1}$	☑
Kglc			1.192	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
Ki			0.910	dimensionless	☑
shock			8.000	dimensionless	☑

8.3 Reaction hxk

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

Name hexokinase

SBO:0000176 biochemical reaction

Reaction equation

$$\mathrm{glc} + \mathrm{atp} \xrightarrow{\mathrm{t6p}} \mathrm{g6p} + \mathrm{adp} + \mathrm{h} \tag{11}$$

Reactants

Table 12: Properties of each reactant.

Id	Name	SBO
glc	glucose	
atp	ATP	

Modifier

Table 13: Properties of each modifier.

Id	Name	SBO
t6p	trehalose 6-phosphate	

Products

Table 14: Properties of each product.

Id	Name	SBO
g6p	glucose 6-phosphate	
adp	ADP	
h	H+	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \frac{\frac{\text{vol(cell)} \cdot \text{shock}^{\text{heat}} \cdot \text{Vmax}}{\text{Kglc} \cdot \text{Katp}} \cdot \left([\text{glc}] \cdot [\text{atp}] - \frac{[\text{g6p}] \cdot [\text{adp}]}{\text{Keq}} \right)}{\left(1 + \frac{[\text{glc}]}{\text{Kglc}} + \frac{[\text{g6p}]}{\text{Kg6p}} + \frac{[\text{t6p}]}{\text{Kit6p}} \right) \cdot \left(1 + \frac{[\text{atp}]}{\text{Katp}} + \frac{[\text{adp}]}{\text{Kadp}} \right)} \tag{12}$$

Table 15: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax			289.60	$\text{mmol} \cdot \text{l}^{-1} \cdot (60\ \text{s})^{-1}$	☑
Kglc			0.08	$\text{mmol} \cdot \text{l}^{-1}$	☑
Katp			0.15	$\text{mmol} \cdot \text{l}^{-1}$	☑
Kg6p			30.00	$\text{mmol} \cdot \text{l}^{-1}$	☑
Kadp			0.23	$\text{mmol} \cdot \text{l}^{-1}$	☑
Keq			2000.00	dimensionless	☑
Kit6p			0.04	$\text{mmol} \cdot \text{l}^{-1}$	☑
shock			8.00	dimensionless	☑

8.4 Reaction pgm

This is a reversible reaction of one reactant forming one product.

Name phosphoglucomutase

SBO:0000176 biochemical reaction

Reaction equation

$$\text{g6p} \rightleftharpoons \text{g1p} \tag{13}$$

Reactant

Table 16: Properties of each reactant.

Id	Name	SBO
g6p	glucose 6-phosphate	

Product

Table 17: Properties of each product.

Id	Name	SBO
g1p	glucose 1-phosphate	

Id	Name	SBO

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \frac{\frac{\text{vol(cell)} \cdot \text{shock}^{\text{heat}} \cdot \text{Vmax}}{\text{Kg6p}} \cdot \left([\text{g6p}] - \frac{[\text{g1p}]}{\text{Keq}} \right)}{1 + \frac{[\text{g6p}]}{\text{Kg6p}} + \frac{[\text{g1p}]}{\text{Kg1p}}} \tag{14}$$

Table 18: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
`Vmax`			0.355	$\text{mmol} \cdot \text{l}^{-1} \cdot (60\ \text{s})^{-1}$	☑
`Kg6p`			0.050	$\text{mmol} \cdot \text{l}^{-1}$	☑
`Kg1p`			0.023	$\text{mmol} \cdot \text{l}^{-1}$	☑
`Keq`			0.167	dimensionless	☑
`shock`			16.000	dimensionless	☑

8.5 Reaction `tpp`

This is an irreversible reaction of two reactants forming two products.

Name T6P phosphatase

SBO:0000176 biochemical reaction

Reaction equation

$$\text{t6p} + \text{h2o} \longrightarrow \text{trh} + \text{pho} \tag{15}$$

Reactants

Table 19: Properties of each reactant.

Id	Name	SBO
`t6p`	trehalose 6-phosphate	
`h2o`	water	

Products

Table 20: Properties of each product.

Id	Name	SBO
trh	trehalose	
pho	phosphate	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \frac{\frac{\text{vol(cell)} \cdot \text{shock}^{\text{heat}} \cdot \text{Vmax} \cdot [\text{t6p}]}{\text{Kt6p}}}{1 + \frac{[\text{t6p}]}{\text{Kt6p}}} \tag{16}$$

Table 21: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax			6.5	$\text{mmol} \cdot \text{l}^{-1} \cdot (60\ \text{s})^{-1}$	☑
Kt6p			0.5	$\text{mmol} \cdot \text{l}^{-1}$	☑
shock			18.0	dimensionless	☑

8.6 Reaction tps

This is an irreversible reaction of two reactants forming three products.

Name T6P synthase

SBO:0000176 biochemical reaction

Reaction equation

$$\text{g6p} + \text{udg} \longrightarrow \text{t6p} + \text{udp} + \text{h} \tag{17}$$

Reactants

Table 22: Properties of each reactant.

Id	Name	SBO
g6p	glucose 6-phosphate	
udg	UDP glucose	

Products

Table 23: Properties of each product.

Id	Name	SBO
t6p	trehalose 6-phosphate	
udp	UDP	
h	H+	

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \frac{\frac{\mathrm{vol(cell)} \cdot \mathrm{activity} \cdot \mathrm{shock}^{\mathrm{heat}} \cdot \mathrm{Vmax} \cdot [\mathrm{g6p}] \cdot [\mathrm{udg}]}{\mathrm{Kg6p} \cdot \mathrm{Kudg}}}{\left(1 + \frac{[\mathrm{g6p}]}{\mathrm{Kg6p}}\right) \cdot \left(1 + \frac{[\mathrm{udg}]}{\mathrm{Kudg}}\right)} \tag{18}$$

Table 24: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax			1.371	$\mathrm{mmol} \cdot \mathrm{l}^{-1} \cdot (60\ \mathrm{s})^{-1}$	☑
Kg6p			3.800	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
Kudg			0.886	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
shock			12.000	dimensionless	☑
activity			1.000	dimensionless	☑

8.7 Reaction nth

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

Name trehalase

SBO:0000176 biochemical reaction

Reaction equation

$$\mathrm{trh} + \mathrm{h2o} \longrightarrow 2\,\mathrm{glc} \tag{19}$$

Reactants

Table 25: Properties of each reactant.

Id	Name	SBO
trh	trehalose	
h2o	water	

Product

Table 26: Properties of each product.

Id	Name	SBO
glc	glucose	

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \frac{\frac{\mathrm{vol(cell)} \cdot \mathrm{shock}^{\mathrm{heat}} \cdot \mathrm{Vmax} \cdot [\mathrm{trh}]}{\mathrm{Ktrh}}}{1 + \frac{[\mathrm{trh}]}{\mathrm{Ktrh}}} \tag{20}$$

Table 27: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax			15.20	$\mathrm{mmol} \cdot \mathrm{l}^{-1} \cdot (60\ \mathrm{s})^{-1}$	☑
Ktrh			2.99	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
shock			6.00	dimensionless	☑

8.8 Reaction ugp

This is an irreversible reaction of three reactants forming two products.

Name UDP glucose phosphorylase

SBO:0000176 biochemical reaction

Reaction equation

$$\mathrm{g1p} + \mathrm{utp} + \mathrm{h} \longrightarrow \mathrm{udg} + \mathrm{ppi} \tag{21}$$

Reactants

Table 28: Properties of each reactant.

Id	Name	SBO
g1p	glucose 1-phosphate	
utp	UTP	
h	H+	

Products

Table 29: Properties of each product.

Id	Name	SBO
udg	UDP glucose	
ppi	diphosphate	

Kinetic Law

Derived unit $0.0010000000000000013\ \mathrm{mol} \cdot (60\ \mathrm{s})^{-1}$

$$v_8 = \frac{\frac{\mathrm{vol(cell)} \cdot \mathrm{shock}^{\mathrm{heat}} \cdot \mathrm{Vmax} \cdot [\mathrm{utp}] \cdot [\mathrm{g1p}]}{\mathrm{Kutp} \cdot \mathrm{Kg1p}}}{\frac{\mathrm{Kiutp}}{\mathrm{Kutp}} + \frac{[\mathrm{utp}]}{\mathrm{Kutp}} + \frac{[\mathrm{g1p}]}{\mathrm{Kg1p}} + \frac{[\mathrm{utp}] \cdot [\mathrm{g1p}]}{\mathrm{Kutp} \cdot \mathrm{Kg1p}} + \frac{\frac{\mathrm{Kiutp}}{\mathrm{Kutp}} \cdot [\mathrm{udg}]}{\mathrm{Kiudg}} + \frac{[\mathrm{g1p}] \cdot [\mathrm{udg}]}{\mathrm{Kg1p} \cdot \mathrm{Kiudg}}} \tag{22}$$

Table 30: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax			36.820	$\mathrm{mmol} \cdot \mathrm{l}^{-1} \cdot (60\ \mathrm{s})^{-1}$	☑
Kutp			0.110	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
Kiutp			0.110	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
Kg1p			0.320	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
Kiudg			0.004	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
shock			16.000	dimensionless	☑

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.

9.1 Species glc

Name glucose

SBO:0000247 simple chemical

Initial concentration $0.09675\ \text{mmol} \cdot \text{l}^{-1}$

Initial assignment glc

This species takes part in three reactions (as a reactant in hxk and as a product in hxt, nth).

$$\frac{\text{d}}{\text{d}t}\text{glc} = v_2 + 2v_7 - v_3 \tag{23}$$

9.2 Species g1p

Name glucose 1-phosphate

SBO:0000247 simple chemical

Initial concentration $0.1\ \text{mmol} \cdot \text{l}^{-1}$

Initial assignment g1p

This species takes part in two reactions (as a reactant in ugp and as a product in pgm).

$$\frac{\text{d}}{\text{d}t}\text{g1p} = v_4 - v_8 \tag{24}$$

9.3 Species g6p

Name glucose 6-phosphate

SBO:0000247 simple chemical

Initial concentration $2.675\ \text{mmol} \cdot \text{l}^{-1}$

Initial assignment g6p

This species takes part in four reactions (as a reactant in pgi, pgm, tps and as a product in hxk).

$$\frac{\text{d}}{\text{d}t}\text{g6p} = v_3 - v_1 - v_4 - v_6 \tag{25}$$

9.4 Species trh

Name trehalose

SBO:0000247 simple chemical

Initial concentration $0.05\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

Initial assignment trh

This species takes part in two reactions (as a reactant in nth and as a product in tpp).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{trh} = v_5 - v_7 \tag{26}$$

9.5 Species t6p

Name trehalose 6-phosphate

SBO:0000247 simple chemical

Initial concentration $0.02\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

Initial assignment t6p

This species takes part in three reactions (as a reactant in tpp and as a product in tps and as a modifier in hxk).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{t6p} = v_6 - v_5 \tag{27}$$

9.6 Species udg

Name UDP glucose

SBO:0000247 simple chemical

Initial concentration $0.7\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

Initial assignment udg

This species takes part in two reactions (as a reactant in tps and as a product in ugp).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{udg} = v_8 - v_6 \tag{28}$$

9.7 Species adp

Name ADP

SBO:0000247 simple chemical

Initial concentration $1.282\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in one reaction (as a product in hxk), which does not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{adp} = 0 \tag{29}$$

9.8 Species atp

Name ATP

SBO:0000247 simple chemical

Initial concentration $2.525\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in one reaction (as a reactant in hxk), which does not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{atp} = 0 \tag{30}$$

9.9 Species ppi

Name diphosphate

SBO:0000247 simple chemical

This species takes part in one reaction (as a product in ugp), which does not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ppi} = 0 \tag{31}$$

9.10 Species f6p

Name fructose 6-phosphate

SBO:0000247 simple chemical

Initial concentration $0.625\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in one reaction (as a product in pgi), which does not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{f6p} = 0 \tag{32}$$

9.11 Species h

Name H+

SBO:0000247 simple chemical

This species takes part in three reactions (as a reactant in ugp and as a product in hxk, tps), which do not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{h} = 0 \tag{33}$$

9.12 Species pho

Name phosphate

SBO:0000247 simple chemical

This species takes part in one reaction (as a product in tpp), which does not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{pho} = 0 \tag{34}$$

9.13 Species udp

Name UDP

SBO:0000247 simple chemical

Initial concentration $0.2815\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in one reaction (as a product in tps), which does not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{udp} = 0 \tag{35}$$

9.14 Species utp

Name UTP

SBO:0000247 simple chemical

Initial concentration $0.6491\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in one reaction (as a reactant in ugp), which does not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{utp} = 0 \tag{36}$$

9.15 Species h2o

Name water

SBO:0000247 simple chemical

This species takes part in two reactions (as a reactant in tpp, nth), which do not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{h2o} = 0 \tag{37}$$

9.16 Species glx

Name glucose

SBO:0000247 simple chemical

Initial concentration $100\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in one reaction (as a reactant in hxt), which does not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{glx} = 0 \tag{38}$$

A Glossary of Systems Biology Ontology Terms

SBO:0000176 biochemical reaction: An event involving one or more chemical entities that modifies the electrochemical structure of at least one of the participants.

SBO:0000185 transport reaction: Movement of a physical entity without modification of the structure of the entity

SBO:0000247 simple chemical: Simple, non-repetitive chemical entity

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