SBML Model Report

Model name: "Ralser2007_Carbohydrate_Rerouting_ROS"

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: Jacky L Snoep[1] and Kieran Smallbone[2] at April eleventh 2007 at 11:09 a. m. and last time modified at February 14th 2014 at 2:48 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	2
species types	0	species	31
events	0	constraints	0
reactions	25	function definitions	0
global parameters	4	unit definitions	5
rules	1	initial assignments	0

Model Notes

This is the model with unfitted parameters described in the article
Dynamic rerouting of the carbohydrate flux is key to counteracting oxidative stress
Markus Ralser, Mirjam M Wamelink, Axel Kowald, Birgit Gerisch, Gino Heeren, Eduard A Struys, Edda Klipp, Cornelis Jakobs, Michael Breitenbach, Hans Lehrach and Sylvia Krobitsch,

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J Biol 2007 6(4):10; PMID: 18154684 , doi: 10.1186/jbiol61
Abstract:
BACKGROUND: Eukaryotic cells have evolved various response mechanisms to counteract the deleterious consequences of oxidative stress. Among these processes, metabolic alterations seem to play an important role.
RESULTS: We recently discovered that yeast cells with reduced activity of the key glycolytic enzyme triosephosphate isomerase exhibit an increased resistance to the thiol-oxidizing reagent diamide. Here we show that this phenotype is conserved in Caenorhabditis elegans and that the underlying mechanism is based on a redirection of the metabolic flux from glycolysis to the pentose phosphate pathway, altering the redox equilibrium of the cytoplasmic NADP(H) pool. Remarkably, another key glycolytic enzyme, glyceraldehyde-3-phosphate dehydrogenase (GAPDH), is known to be inactivated in response to various oxidant treatments, and we show that this provokes a similar redirection of the metabolic flux.
CONCLUSION: The naturally occurring inactivation of GAPDH functions as a metabolic switch for rerouting the carbohydrate flux to counteract oxidative stress. As a consequence, altering the homoeostasis of cytoplasmic metabolites is a fundamental mechanism for balancing the redox state of eukaryotic cells under stress conditions.

Different realtive enzyme velocities can be simulated by varying the parameters **k_rel_TPI** and **k_rel_GAPDH** .

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 millimole

Definition mmol

2.2 Unit `time`

Name minute

Definition 60 s

2.3 Unit mMpermin

Name mMpermin

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

2.4 Unit mM

Name mM

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

2.5 Unit permin

Name permin

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

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
`extracellular`	extracellular	0000290	3	1	litre	☑	
`cytoplasm`	cytoplasm		3	1	litre	☑	`extracellular`

3.1 Compartment `extracellular`

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

Name extracellular

SBO:0000290 physical compartment

3.2 Compartment `cytoplasm`

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

Name cytoplasm

4 Species

This model contains 31 species. The boundary condition of seven of these species is set to `true` so that these species' amount cannot be changed by any reaction. 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
P	High energy phosphates	cytoplasm	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
G6P	Glucose 6 Phosphate	cytoplasm	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
F6P	Fructose 6 Phosphate	cytoplasm	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
F16P	Fructose-1,6 bisphosphate	cytoplasm	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
NADH	NADH	cytoplasm	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
NAD	NAD	cytoplasm	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
BPG	1,3-bisphosphoglycerate	cytoplasm	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
P3G	3-phosphoglycerate	cytoplasm	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
P2G	2-phosphoglycerate	cytoplasm	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
PEP	Phosphoenolpyruvate	cytoplasm	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
PYR	Pyruvate	cytoplasm	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
ACE	Acetaldehyde	cytoplasm	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
CO2	CO2	extracellular	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	☑
ETOH	Ethanol	extracellular	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	☑
SUCC	Succinate	extracellular	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	☑
X	X	cytoplasm	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	☑
GA3P	glyceraldehyde 3-phosphate	cytoplasm	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
DHAP	dihydroxyacetone phosphate	cytoplasm	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
GLY	Glycerol	extracellular	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	☑
D6PGluconoLactone	D-6-phosphoglucono-delta-lactone	cytoplasm	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
D6PGluconate	6-phosphogluconate	cytoplasm	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟

Id	Name	Compartment	Derived Unit	Constant	Boundary Condition
NADP	NADP+	cytoplasm	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
NADPH	NADPH	cytoplasm	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Ribulose5P	ribulose 5-phosphate	cytoplasm	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Ribose5P	ribose 5-phosphate	cytoplasm	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Xyl5P	xylulose 5-phosphate	cytoplasm	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Seduhept7P	sedoheptulose 7-phosphate	cytoplasm	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Erythrose4P	erythrose 4-phosphate	cytoplasm	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
GLCo	Extracellular Glucose	extracellular	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	☑
GLCi	Glucose in Cytosol	cytoplasm	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
F26BP	F2,6P	cytoplasm	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	☑

5 Parameters

This model contains four global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k_rel_TPI	k_rel_TPI		1.0	dimensionless	☑
k_rel_GAPDH	k_rel_GAPDH		1.0	dimensionless	☑
ratio_NADPH-_NADP	ratio_NADPH-_NADP		0.0	dimensionless	☐
SUMAXP	sum of AXP conc		4.1		☑

6 Rule

This is an overview of one rule.

6.1 Rule ratio_NADPH_NADP

Rule ratio_NADPH_NADP is an assignment rule for parameter ratio_NADPH_NADP:

$$\text{ratio\_NADPH\_NADP} = \frac{[\text{NADPH}]}{[\text{NADP}]} \tag{1}$$

Derived unit dimensionless

7 Reactions

This model contains 25 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	vGLK	Hexokinase	$GLCi + P \rightleftharpoons G6P$	0000216
2	vPGI	Glucose-6-phosphate isomerase	$G6P \rightleftharpoons F6P$	0000377
3	vPFK	Phosphofructokinase	$F6P + P \overset{F26BP}{\rightleftharpoons} F16P$	0000216
4	vALD	Aldolase	$F16P \rightleftharpoons DHAP + GA3P$	0000182
5	vG3PDH	Glycerol 3-phosphate dehydrogenase	$DHAP + NADH \rightleftharpoons GLY + NAD$	0000200
6	vGAPDH	Glyceraldehyde 3-phosphate dehydrogenase	$GA3P + NAD \rightleftharpoons BPG + NADH$	0000200
7	vPGK	Phosphoglycerate kinase	$BPG \rightleftharpoons P3G + P$	0000216
8	vPGM	Phosphoglycerate mutase	$P3G \rightleftharpoons P2G$	0000377
9	vENO	Enolase	$P2G \rightleftharpoons PEP$	0000211
10	vPYK	Pyruvate kinase	$PEP \rightleftharpoons PYR + P$	0000216
11	vPDC	Pyruvate decarboxylase	$PYR \rightleftharpoons ACE + CO2$	0000399
12	vSUC	Succinate synthesis	$2\,ACE + 3\,NAD \rightleftharpoons 3\,NADH + SUCC$	0000205
13	vADH	Alcohol dehydrogenase	$ACE + NADH \rightleftharpoons ETOH + NAD$	0000200
14	vATP	ATPase activity	$P \rightleftharpoons X$	0000376
15	vTPI	vTPI	$GA3P \rightleftharpoons DHAP$	0000377
16	vG6PDH	vG6PDH	$G6P + NADP \overset{NADPH}{\longrightarrow} D6PGluconoLactone + NADPH$	0000200
17	v6PGL	v6PGL	$D6PGluconoLactone \longrightarrow D6PGluconate$	0000376
18	vGluDH	vGluDH	$D6PGluconate + NADP \overset{NADPH}{\longrightarrow} Ribulose5P + NADPH$	0000200
19	vPPI	vPPI	$Ribulose5P \rightleftharpoons Ribose5P$	0000377
20	vTransk1	vTransk1	$Ribose5P + Xyl5P \rightleftharpoons GA3P + Seduhept7P$	0000182

№	Id	Name	Reaction Equation	SBO
21	vR5PI	vR5PI	Ribulose5P $\rightleftharpoons$ Xyl5P	0000377
22	vTransald	vTransald	Seduhept7P + GA3P $\rightleftharpoons$ F6P + Erythrose4P	0000182
23	vTransk2	vTransk2	Xyl5P + Erythrose4P $\rightleftharpoons$ GA3P + F6P	0000182
24	vNADPH	vNADPH	NADPH $\longrightarrow$ NADP	0000201
25	vGLT	Glucose transport	GLCo $\rightleftharpoons$ GLCi	0000185

7.1 Reaction vGLK

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

Name Hexokinase

SBO:0000216 phosphorylation

Reaction equation

$$\mathrm{GLCi} + \mathrm{P} \rightleftharpoons \mathrm{G6P} \tag{2}$$

Reactants

Table 6: Properties of each reactant.

Id	Name	SBO
GLCi	Glucose in Cytosol	
P	High energy phosphates	

Product

Table 7: Properties of each product.

Id	Name	SBO
G6P	Glucose 6 Phosphate	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \mathrm{vol}\,(\mathrm{cytoplasm}) \cdot \frac{\mathrm{VmGLK} \cdot \left(\left(\frac{[\mathrm{G6P}] \cdot \left(\mathrm{SUMAXP} - \left(\mathrm{SUMAXP}^2 - 2 \cdot \mathrm{SUMAXP} \cdot [\mathrm{P}] + 8 \cdot \mathrm{KeqAK} \cdot \mathrm{SUMAXP} \cdot [\mathrm{P}] + [\mathrm{P}]^2 - 4 \cdot \mathrm{KeqAK} \cdot [\mathrm{P}]^2\right)^{0.5}\right)}{(1 - 4 \cdot \mathrm{KeqAK}) \cdot \mathrm{KeqGLK}}\right)\right.}{\mathrm{KmGLKATP} \cdot \mathrm{KmGLKGLCi} \cdot \left(1 + \frac{[\mathrm{G6P}]}{\mathrm{KmGLKG6P}} + \frac{[\mathrm{GLCi}]}{\mathrm{KmGLKGLCi}}\right) \cdot \left(1 + \frac{\mathrm{SUMAXP} - \left(\mathrm{SUMAXP}^2 - 2 \cdot \mathrm{SUMAXP} \cdot [\mathrm{P}] + 8 \cdot \mathrm{KeqAK} \cdot \mathrm{S}\right.\right.}{(1 - 4 \cdot \mathrm{KeqAK}) \cdot \mathrm{KmGL}} \tag{3}$$

Table 8: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
VmGLK			226.452	$\mathrm{mmol} \cdot \mathrm{l}^{-1} \cdot (60\ \mathrm{s})^{-1}$	☑

Id	Name	SBO	Value	Unit	Constant
KeqAK			0.450	dimensionless	☑
KeqGLK			3800.000	dimensionless	☑
KmGLKATP			0.150	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KmGLKGLCi			0.080	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KmGLKG6P			30.000	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KmGLKADP			0.230	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑

7.2 Reaction vPGI

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

Name Glucose-6-phosphate isomerase

SBO:0000377 isomerisation

Reaction equation

$$\mathrm{G6P} \rightleftharpoons \mathrm{F6P} \tag{4}$$

Reactant

Table 9: Properties of each reactant.

Id	Name	SBO
G6P	Glucose 6 Phosphate	

Product

Table 10: Properties of each product.

Id	Name	SBO
F6P	Fructose 6 Phosphate	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \mathrm{vol}\,(\mathrm{cytoplasm}) \cdot \frac{\frac{\mathrm{VmPGI}}{\mathrm{KmPGIG6P}} \cdot \left([\mathrm{G6P}] - \frac{[\mathrm{F6P}]}{\mathrm{KeqPGI}}\right)}{1 + \frac{[\mathrm{G6P}]}{\mathrm{KmPGIG6P}} + \frac{[\mathrm{F6P}]}{\mathrm{KmPGIF6P}}} \tag{5}$$

Table 11: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
VmPGI			339.677	mmol · l^{-1} · $(60\ s)^{-1}$	☑
KmPGIG6P			1.400	mmol · l^{-1}	☑
KeqPGI			0.314	dimensionless	☑
KmPGIF6P			0.300	mmol · l^{-1}	☑

7.3 Reaction vPFK

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

Name Phosphofructokinase

SBO:0000216 phosphorylation

Reaction equation

$$\mathrm{F6P} + \mathrm{P} \overset{\mathrm{F26BP}}{\rightleftharpoons} \mathrm{F16P} \tag{6}$$

Reactants

Table 12: Properties of each reactant.

Id	Name	SBO
F6P	Fructose 6 Phosphate	
P	High energy phosphates	

Modifier

Table 13: Properties of each modifier.

Id	Name	SBO
F26BP	F2,6P	

Product

Table 14: Properties of each product.

Id	Name	SBO
F16P	Fructose-1,6 bisphosphate	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \mathrm{vol}\,(\mathrm{cytoplasm}) \tag{7}$$

$$\cdot \frac{\mathrm{gR} \cdot \mathrm{VmPFK} \cdot [\mathrm{F6P}] \cdot}{(2 - 8 \cdot \mathrm{KeqAK}) \cdot \mathrm{KmPFKATP} \cdot \mathrm{KmPFKF6P} \cdot \left(\mathrm{L0} \cdot \left(1 + \frac{\mathrm{CPFKF26BP} \cdot [\mathrm{F26BP}]}{\mathrm{KPFKF26BP}} + \frac{\mathrm{CPFKF16BP} \cdot [\mathrm{F16P}]}{\mathrm{KPFKF16BP}}\right)^2 \cdot \left(1 + \frac{2 \cdot \mathrm{CPFKAMP} \cdot \mathrm{KeqAK} \cdot (\mathrm{SUM}}{(-1+4 \cdot \mathrm{KeqAK}) \cdot \mathrm{KPFKAMP} \cdot (\mathrm{SUMAXP}-} \right.}{\left. \left(1 + \frac{[\mathrm{F26BP}]}{\mathrm{KPFKF26BP}} + \right. \right.}$$

Table 15: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
gR			5.120	dimensionless	☑
VmPFK			182.903	$\mathrm{mmol} \cdot \mathrm{l}^{-1} \cdot (60\ \mathrm{s})^{-1}$	☑
KeqAK			0.450	dimensionless	☑
KmPFKF6P			0.100	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KmPFKATP			0.710	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
L0			0.660	dimensionless	☑
CPFKF26BP			0.017	dimensionless	☑
KPFKF26BP			$6.82 \cdot 10^{-4}$	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
CPFKF16BP			0.397	dimensionless	☑
KPFKF16BP			0.111	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
CPFKAMP			0.085	dimensionless	☑
KPFKAMP			0.100	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
CiPFKATP			100.000	dimensionless	☑
KiPFKATP			0.650	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
CPFKATP			3.000	dimensionless	☑

7.4 Reaction vALD

This is a reversible reaction of one reactant forming two products.

Name Aldolase

SBO:0000182 conversion

Reaction equation

$$\mathrm{F16P} \rightleftharpoons \mathrm{DHAP} + \mathrm{GA3P} \tag{8}$$

Reactant

Table 16: Properties of each reactant.

Id	Name	SBO
F16P	Fructose-1,6 bisphosphate	

Products

Table 17: Properties of each product.

Id	Name	SBO
DHAP	dihydroxyacetone phosphate	
GA3P	glyceraldehyde 3-phosphate	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \mathrm{vol}\,(\mathrm{cytoplasm}) \cdot \frac{\frac{\mathrm{VmALD}\cdot[\mathrm{F16P}]}{\mathrm{KmALDF16P}} \cdot \left(1 - \frac{[\mathrm{DHAP}]\cdot[\mathrm{GA3P}]}{[\mathrm{F16P}]\cdot\mathrm{KeqALD}}\right)}{1 + \frac{[\mathrm{F16P}]}{\mathrm{KmALDF16P}} + \frac{[\mathrm{DHAP}]}{\mathrm{KmALDDHAP}} + \frac{[\mathrm{GA3P}]}{\mathrm{KmALDGAP}} + \frac{[\mathrm{F16P}]\cdot[\mathrm{GA3P}]}{\mathrm{KmALDF16P}\cdot\mathrm{KmALDGAPi}} + \frac{[\mathrm{DHAP}]\cdot[\mathrm{GA3P}]}{\mathrm{KmALDDHAP}\cdot\mathrm{KmALDGAP}}} \tag{9}$$

Table 18: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
VmALD			322.258	$\mathrm{mmol}\cdot\mathrm{l}^{-1}\cdot(60\ \mathrm{s})^{-1}$	☑
KeqTPI			0.045	dimensionless	☑
KeqALD			0.069	dimensionless	☑
KmALDF16P			0.300	$\mathrm{mmol}\cdot\mathrm{l}^{-1}$	☑
KmALDDHAP			2.400	$\mathrm{mmol}\cdot\mathrm{l}^{-1}$	☑
KmALDGAP			2.000	$\mathrm{mmol}\cdot\mathrm{l}^{-1}$	☑
KmALDGAPi			10.000	$\mathrm{mmol}\cdot\mathrm{l}^{-1}$	☑

7.5 Reaction vG3PDH

This is a reversible reaction of two reactants forming two products.

Name Glycerol 3-phosphate dehydrogenase

SBO:0000200 redox reaction

Reaction equation

$$\mathrm{DHAP} + \mathrm{NADH} \rightleftharpoons \mathrm{GLY} + \mathrm{NAD} \tag{10}$$

Reactants

Table 19: Properties of each reactant.

Id	Name	SBO
DHAP	dihydroxyacetone phosphate	
NADH	NADH	

Products

Table 20: Properties of each product.

Id	Name	SBO
GLY	Glycerol	
NAD	NAD	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \mathrm{vol}\,(\mathrm{cytoplasm}) \cdot \frac{\mathrm{VmG3PDH} \cdot \left(\left(\frac{[\mathrm{GLY}] \cdot [\mathrm{NAD}]}{\mathrm{KeqG3PDH}} \right) + \frac{[\mathrm{NADH}] \cdot [\mathrm{DHAP}]}{1 + \mathrm{KeqTPI}} \right)}{\mathrm{KmG3PDHDHAP} \cdot \mathrm{KmG3PDHNADH} \cdot \left(1 + \frac{[\mathrm{NAD}]}{\mathrm{KmG3PDHNAD}} + \frac{[\mathrm{NADH}]}{\mathrm{KmG3PDHNADH}} \right) \cdot \left(1 + \frac{[\mathrm{GLY}]}{\mathrm{KmG3PDHGLY}} + \frac{[}{(1+\mathrm{KeqTPI})} \right.} \tag{11}$$

Table 21: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
VmG3PDH			70.150	$\mathrm{mmol} \cdot \mathrm{l}^{-1} \cdot (60\ \mathrm{s})^{-1}$	☑

Id	Name	SBO	Value	Unit	Constant
KeqG3PDH			4300.000	dimensionless	☑
KeqTPI			0.045	dimensionless	☑
KmG3PDHDHAP			0.400	$\mathrm{mmol}\cdot\mathrm{l}^{-1}$	☑
KmG3PDHNADH			0.023	$\mathrm{mmol}\cdot\mathrm{l}^{-1}$	☑
KmG3PDHNAD			0.930	$\mathrm{mmol}\cdot\mathrm{l}^{-1}$	☑
KmG3PDHGLY			1.000	$\mathrm{mmol}\cdot\mathrm{l}^{-1}$	☑

7.6 Reaction vGAPDH

This is a reversible reaction of two reactants forming two products.

Name Glyceraldehyde 3-phosphate dehydrogenase

SBO:0000200 redox reaction

Reaction equation

$$\mathrm{GA3P} + \mathrm{NAD} \rightleftharpoons \mathrm{BPG} + \mathrm{NADH} \tag{12}$$

Reactants

Table 22: Properties of each reactant.

Id	Name	SBO
GA3P	glyceraldehyde 3-phosphate	
NAD	NAD	

Products

Table 23: Properties of each product.

Id	Name	SBO
BPG	1,3-bisphosphoglycerate	
NADH	NADH	

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \mathrm{vol}\,(\mathrm{cytoplasm}) \cdot \frac{\frac{\mathrm{k\_rel\_GAPDH} \cdot \mathrm{VmGAPDHf} \cdot [\mathrm{GA3P}] \cdot [\mathrm{NAD}]}{\mathrm{KmGAPDHGAP} \cdot \mathrm{KmGAPDHNAD}} \cdot \left(1 - \frac{[\mathrm{BPG}] \cdot [\mathrm{NADH}]}{[\mathrm{GA3P}] \cdot [\mathrm{NAD}] \cdot \mathrm{KeqGAPDH}}\right)}{\left(1 + \frac{[\mathrm{GA3P}]}{\mathrm{KmGAPDHGAP}} + \frac{[\mathrm{BPG}]}{\mathrm{KmGAPDHBPG}}\right) \cdot \left(1 + \frac{[\mathrm{NAD}]}{\mathrm{KmGAPDHNAD}} + \frac{[\mathrm{NADH}]}{\mathrm{KmGAPDHNADH}}\right)} \tag{13}$$

Table 24: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
VmGAPDHr			6549.680	$\mathrm{mmol} \cdot \mathrm{l}^{-1} \cdot (60\ \mathrm{s})^{-1}$	☑
KmGAPDHBPG			0.010	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KmGAPDHNADH			0.060	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KeqTPI			0.045	dimensionless	☑
VmGAPDHf			1184.520	$\mathrm{mmol} \cdot \mathrm{l}^{-1} \cdot (60\ \mathrm{s})^{-1}$	☑
KmGAPDHGAP			0.210	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KmGAPDHNAD			0.090	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KeqGAPDH	KeqGAPDH		0.005	dimensionless	☑

7.7 Reaction vPGK

This is a reversible reaction of one reactant forming two products.

Name Phosphoglycerate kinase

SBO:0000216 phosphorylation

Reaction equation

$$\mathrm{BPG} \rightleftharpoons \mathrm{P3G} + \mathrm{P} \tag{14}$$

Reactant

Table 25: Properties of each reactant.

Id	Name	SBO
BPG	1,3-bisphosphoglycerate	

Products

Table 26: Properties of each product.

Id	Name	SBO
P3G	3-phosphoglycerate	
P	High energy phosphates	

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \mathrm{vol}\,(\mathrm{cytoplasm}) \cdot \frac{\mathrm{VmPGK} \cdot \left(\frac{\mathrm{KeqPGK}\cdot[\mathrm{BPG}]\cdot\left(\mathrm{SUMAXP}-\left(\mathrm{SUMAXP}^2-2\cdot\mathrm{SUMAXP}\cdot[\mathrm{P}]+8\cdot\mathrm{KeqAK}\cdot\mathrm{SUMAXP}\cdot[\mathrm{P}]+[\mathrm{P}]^2-4\cdot\mathrm{KeqAK}\cdot[\mathrm{P}]^2\right)^{0.}\right.}{1-4\cdot\mathrm{KeqAK}} \right.}{\mathrm{KmPGKATP}\cdot\mathrm{KmPGKP3G}\cdot\left(1+\frac{\mathrm{SUMAXP}-\left(\mathrm{SUMAXP}^2-2\cdot\mathrm{SUMAXP}\cdot[\mathrm{P}]+8\cdot\mathrm{KeqAK}\cdot\mathrm{SUMAXP}\cdot[\mathrm{P}]+[\mathrm{P}]^2-4\cdot\mathrm{KeqAK}\cdot[\mathrm{P}]^2\right)^{0.5}}{(1-4\cdot\mathrm{KeqAK})\cdot\mathrm{KmPGKADP}}+\frac{\mathrm{SU}}{} \right.} \tag{15}$$

Table 27: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
VmPGK			1306.450	$\mathrm{mmol}\cdot 1^{-1}\cdot(60\ \mathrm{s})^{-1}$	☑
KeqPGK			3200.000	dimensionless	☑
KeqAK			0.450	dimensionless	☑
KmPGKATP			0.300	$\mathrm{mmol}\cdot 1^{-1}$	☑
KmPGKP3G			0.530	$\mathrm{mmol}\cdot 1^{-1}$	☑
KmPGKADP			0.200	$\mathrm{mmol}\cdot 1^{-1}$	☑
KmPGKBPG			0.003	$\mathrm{mmol}\cdot 1^{-1}$	☑

7.8 Reaction vPGM

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

Name Phosphoglycerate mutase

SBO:0000377 isomerisation

Reaction equation

$$\mathrm{P3G} \rightleftharpoons \mathrm{P2G} \tag{16}$$

Reactant

Table 28: Properties of each reactant.

Id	Name	SBO
P3G	3-phosphoglycerate	

Product

Table 29: Properties of each product.

Id	Name	SBO
P2G	2-phosphoglycerate	

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \mathrm{vol}\,(\mathrm{cytoplasm}) \cdot \frac{\frac{\mathrm{VmPGM}}{\mathrm{KmPGMP3G}} \cdot \left([\mathrm{P3G}] - \frac{[\mathrm{P2G}]}{\mathrm{KeqPGM}}\right)}{1 + \frac{[\mathrm{P3G}]}{\mathrm{KmPGMP3G}} + \frac{[\mathrm{P2G}]}{\mathrm{KmPGMP2G}}} \tag{17}$$

Table 30: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
VmPGM			2525.81	$\mathrm{mmol} \cdot \mathrm{l}^{-1} \cdot (60\ \mathrm{s})^{-1}$	☑
KmPGMP3G			1.20	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KeqPGM			0.19	dimensionless	☑
KmPGMP2G			0.08	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑

7.9 Reaction vENO

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

Name Enolase

SBO:0000211 removal of a chemical group

Reaction equation

$$\mathrm{P2G} \rightleftharpoons \mathrm{PEP} \tag{18}$$

Reactant

Table 31: Properties of each reactant.

Id	Name	SBO
P2G	2-phosphoglycerate	

Product

Table 32: Properties of each product.

Id	Name	SBO
PEP	Phosphoenolpyruvate	

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \mathrm{vol}\,(\mathrm{cytoplasm}) \cdot \frac{\frac{\mathrm{VmENO}}{\mathrm{KmENOP2G}} \cdot \left([\mathrm{P2G}] - \frac{[\mathrm{PEP}]}{\mathrm{KeqENO}}\right)}{1 + \frac{[\mathrm{P2G}]}{\mathrm{KmENOP2G}} + \frac{[\mathrm{PEP}]}{\mathrm{KmENOPEP}}} \tag{19}$$

Table 33: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
VmENO			365.806	$\mathrm{mmol} \cdot \mathrm{l}^{-1} \cdot (60\ \mathrm{s})^{-1}$	☑
KmENOP2G			0.040	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KeqENO			6.700	dimensionless	☑
KmENOPEP			0.500	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑

7.10 Reaction vPYK

This is a reversible reaction of one reactant forming two products.

Name Pyruvate kinase

SBO:0000216 phosphorylation

Reaction equation

$$\mathrm{PEP} \rightleftharpoons \mathrm{PYR} + \mathrm{P} \tag{20}$$

Reactant

Table 34: Properties of each reactant.

Id	Name	SBO
PEP	Phosphoenolpyruvate	

Products

Table 35: Properties of each product.

Id	Name	SBO
PYR	Pyruvate	
P	High energy phosphates	

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = \mathrm{vol}\,(\mathrm{cytoplasm}) \tag{21}$$

$$\frac{\mathrm{VmPYK}}{\mathrm{KmPYKPEP}\cdot\mathrm{KmPYKADP}}\cdot\left(\frac{[\mathrm{PEP}]\cdot\left(\mathrm{SUMAXP}-\left([\mathrm{P}]^2-4\cdot\mathrm{KeqAK}\cdot[\mathrm{P}]^2-2\cdot[\mathrm{P}]\cdot\mathrm{SUMAXP}+8\cdot\mathrm{KeqAK}\cdot[\mathrm{P}]\cdot\mathrm{SUMAXP}+\mathrm{SUMAXP}^2\right)^{0.5}\right)}{1-4\cdot\mathrm{KeqAK}}-\frac{[\mathrm{PYR}]\cdot\left([\mathrm{P}]-\right.}{}\right.$$

$$\cdot\frac{}{\left(1+\frac{[\mathrm{PEP}]}{\mathrm{KmPYKPEP}}+\frac{[\mathrm{PYR}]}{\mathrm{KmPYKPYR}}\right)\cdot\left(1+\frac{\frac{[\mathrm{P}]-4\cdot\mathrm{KeqAK}\cdot[\mathrm{P}]-\mathrm{SUMAXP}+\left([\mathrm{P}]^2-4\cdot\mathrm{KeqAK}\cdot[\mathrm{P}]^2-2\cdot[\mathrm{P}]\cdot\mathrm{SUMAXP}+8\cdot\mathrm{KeqAK}\cdot[\mathrm{P}]\cdot\mathrm{SUMAXP}+\mathrm{SUMAXP}^2\right)^{0.5}}{2-8\cdot\mathrm{KeqAK}}}{\mathrm{KmPYKATP}}\right.}$$

Table 36: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
VmPYK			1088.71	$\mathrm{mmol}\cdot 1^{-1}\cdot(60\ \mathrm{s})^{-1}$	☑
KmPYKPEP			0.14	$\mathrm{mmol}\cdot 1^{-1}$	☑
KmPYKADP			0.53	$\mathrm{mmol}\cdot 1^{-1}$	☑
KeqAK			0.45	dimensionless	☑
KeqPYK			6500.00	dimensionless	☑
KmPYKPYR			21.00	$\mathrm{mmol}\cdot 1^{-1}$	☑
KmPYKATP			1.50	$\mathrm{mmol}\cdot 1^{-1}$	☑

7.11 Reaction vPDC

This is a reversible reaction of one reactant forming two products.

Name Pyruvate decarboxylase

SBO:0000399 decarboxylation

Reaction equation

$$\mathrm{PYR} \rightleftharpoons \mathrm{ACE} + \mathrm{CO2} \tag{22}$$

Reactant

Table 37: Properties of each reactant.

Id	Name	SBO
PYR	Pyruvate	

Products

Table 38: Properties of each product.

Id	Name	SBO
ACE	Acetaldehyde	
CO2	CO2	

Kinetic Law

Derived unit contains undeclared units

$$v_{11} = \mathrm{vol}\,(\mathrm{cytoplasm}) \cdot \frac{\frac{\mathrm{VmPDC} \cdot [\mathrm{PYR}]^{\mathrm{nPDC}}}{\mathrm{KmPDCPYR}^{\mathrm{nPDC}}}}{1 + \frac{[\mathrm{PYR}]^{\mathrm{nPDC}}}{\mathrm{KmPDCPYR}^{\mathrm{nPDC}}}} \tag{23}$$

Table 39: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
VmPDC			174.194	$\mathrm{mmol} \cdot \mathrm{l}^{-1} \cdot (60\ \mathrm{s})^{-1}$	☑
nPDC			1.900	dimensionless	☑
KmPDCPYR			4.330	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑

7.12 Reaction vSUC

This is a reversible reaction of two reactants forming two products.

Name Succinate synthesis

SBO:0000205 composite biochemical process

Reaction equation

$$2\,\mathrm{ACE} + 3\,\mathrm{NAD} \rightleftharpoons 3\,\mathrm{NADH} + \mathrm{SUCC} \tag{24}$$

Reactants

Table 40: Properties of each reactant.

Id	Name	SBO
ACE	Acetaldehyde	
NAD	NAD	

Products

Table 41: Properties of each product.

Id	Name	SBO
NADH	NADH	
SUCC	Succinate	

Kinetic Law

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

$$v_{12} = \mathrm{vol}\,(\mathrm{cytoplasm}) \cdot \mathrm{KSUCC} \cdot [\mathrm{ACE}] \tag{25}$$

Table 42: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
KSUCC			21.4	$(60\ \mathrm{s})^{-1}$	☑

7.13 Reaction vADH

This is a reversible reaction of two reactants forming two products.

Name Alcohol dehydrogenase

SBO:0000200 redox reaction

Reaction equation

$$\mathrm{ACE} + \mathrm{NADH} \rightleftharpoons \mathrm{ETOH} + \mathrm{NAD} \tag{26}$$

Reactants

Table 43: Properties of each reactant.

Id	Name	SBO
ACE	Acetaldehyde	
NADH	NADH	

Products

Table 44: Properties of each product.

Id	Name	SBO
ETOH	Ethanol	
NAD	NAD	

Kinetic Law

Derived unit $0.0010\ \mathrm{mol} \cdot (60\ \mathrm{s})^{-1}$

$$v_{13} = \mathrm{vol}(\mathrm{cytoplasm}) \tag{27}$$
$$\cdot \left(\left(\frac{}{1 + \frac{[\mathrm{NAD}]}{\mathrm{KiADHNAD}} + \frac{\mathrm{KmADHNAD} \cdot [\mathrm{ETOH}]}{\mathrm{KiADHNAD} \cdot \mathrm{KmADHETOH}} + \frac{\mathrm{KmADHNADH} \cdot [\mathrm{ACE}]}{\mathrm{KiADHNADH} \cdot \mathrm{KmADHACE}} + \frac{[\mathrm{NADH}]}{\mathrm{KiADHNADH}} + \frac{[\mathrm{NAD}] \cdot [\mathrm{ETOH}]}{\mathrm{KiADHNAD} \cdot \mathrm{KmADHETOH}} +} \right. \right.$$

Table 45: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
VmADH			810.000	$\mathrm{mmol} \cdot \mathrm{l}^{-1} \cdot (60\ \mathrm{s})^{-1}$	☑

Id	Name	SBO	Value	Unit	Constant
KiADHNAD			0.920	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KmADHETOH			17.000	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KeqADH			$6.9 \cdot 10^{-5}$	dimensionless	☑
KmADHNAD			0.170	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KmADHNADH			0.110	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KiADHNADH			0.031	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KmADHACE			1.110	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KiADHACE			1.100	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KiADHETOH			90.000	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑

7.14 Reaction vATP

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

Name ATPase activity

SBO:0000376 hydrolysis

Reaction equation

$$\mathrm{P} \rightleftharpoons \mathrm{X} \tag{28}$$

Reactant

Table 46: Properties of each reactant.

Id	Name	SBO
P	High energy phosphates	

Product

Table 47: Properties of each product.

Id	Name	SBO
X	X	

Kinetic Law

Derived unit contains undeclared units

$$v_{14} = \mathrm{vol}\,(\mathrm{cytoplasm}) \cdot \frac{\mathrm{KATPASE} \cdot \left([\mathrm{P}] - 4 \cdot \mathrm{KeqAK} \cdot [\mathrm{P}] - \mathrm{SUMAXP} + \left([\mathrm{P}]^2 - 4 \cdot \mathrm{KeqAK} \cdot [\mathrm{P}]^2 - 2 \cdot [\mathrm{P}] \cdot \mathrm{SUMAXP} + 8 \cdot \mathrm{KeqAK} \cdot \right.\right.}{2 - 8 \cdot \mathrm{KeqAK}} \tag{29}$$

Table 48: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
KATPASE			39.50	$(60\ \mathrm{s})^{-1}$	☑
KeqAK			0.45	dimensionless	☑

7.15 Reaction vTPI

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

Name vTPI

SBO:0000377 isomerisation

Reaction equation

$$\mathrm{GA3P} \rightleftharpoons \mathrm{DHAP} \tag{30}$$

Reactant

Table 49: Properties of each reactant.

Id	Name	SBO
GA3P	glyceraldehyde 3-phosphate	

Product

Table 50: Properties of each product.

Id	Name	SBO
DHAP	dihydroxyacetone phosphate	

Kinetic Law

Derived unit contains undeclared units

$$v_{15} = \mathrm{vol}\,(\mathrm{cytoplasm}) \cdot \frac{\mathrm{k\_rel\_TPI} \cdot \left(\frac{\mathrm{VmDHAP} \cdot [\mathrm{GA3P}]}{\mathrm{KmGA3P}} - \frac{\mathrm{VmGA3P} \cdot [\mathrm{DHAP}]}{\mathrm{KmDHAP}} \right)}{1 + \frac{[\mathrm{GA3P}]}{\mathrm{KmGA3P}} + \frac{[\mathrm{DHAP}]}{\mathrm{KmDHAP}}} \tag{31}$$

Table 51: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
KmGA3P	KmGA3P		1.27	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KmDHAP	KmDHAP		1.23	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
VmDHAP	VmDHAP		10900.00	$\mathrm{mmol} \cdot \mathrm{l}^{-1} \cdot (60\ \mathrm{s})^{-1}$	☑
VmGA3P	VmGA3P		555.00	$\mathrm{mmol} \cdot \mathrm{l}^{-1} \cdot (60\ \mathrm{s})^{-1}$	☑

7.16 Reaction vG6PDH

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

Name vG6PDH

SBO:0000200 redox reaction

Reaction equation

$$\mathrm{G6P} + \mathrm{NADP} \xrightarrow{\mathrm{NADPH}} \mathrm{D6PGluconoLactone} + \mathrm{NADPH} \tag{32}$$

Reactants

Table 52: Properties of each reactant.

Id	Name	SBO
G6P	Glucose 6 Phosphate	
NADP	NADP+	

Modifier

Table 53: Properties of each modifier.

Id	Name	SBO
NADPH	NADPH	

Products

Table 54: Properties of each product.

Id	Name	SBO
D6PGluconoLactone	D-6-phosphoglucono-delta-lactone	
NADPH	NADPH	

Kinetic Law

Derived unit contains undeclared units

$$v_{16} = \mathrm{vol}\,(\mathrm{cytoplasm}) \cdot \frac{\frac{\mathrm{VmG6PDH} \cdot [\mathrm{G6P}] \cdot [\mathrm{NADP}]}{\mathrm{KmG6P} \cdot \mathrm{KmNADP}}}{\left(1 + \frac{[\mathrm{G6P}]}{\mathrm{KmG6P}} + \frac{[\mathrm{NADPH}]}{\mathrm{KiNADPH}}\right) \cdot \left(1 + \frac{[\mathrm{NADP}]}{\mathrm{KmNADP}}\right)} \tag{33}$$

Table 55: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
VmG6PDH	VmG6PDH		4.000	$\mathrm{mmol} \cdot \mathrm{l}^{-1} \cdot (60\ \mathrm{s})^{-1}$	☑
KmG6P	KmG6P		0.040	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KmNADP	KmNADP		0.020	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KiNADPH	KiNADPH		0.017	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑

7.17 Reaction v6PGL

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

Name v6PGL

SBO:0000376 hydrolysis

Reaction equation

$$\mathrm{D6PGluconoLactone} \longrightarrow \mathrm{D6PGluconate} \tag{34}$$

Reactant

Table 56: Properties of each reactant.

Id	Name	SBO
D6PGluconoLactone	D-6-phosphoglucono-delta-lactone	

Product

Table 57: Properties of each product.

Id	Name	SBO
D6PGluconate	6-phosphogluconate	

Kinetic Law

Derived unit $0.0010\,\mathrm{mol}\cdot(60\,\mathrm{s})^{-1}$

$$v_{17} = \mathrm{vol}\,(\mathrm{cytoplasm}) \cdot \frac{\mathrm{Vm6PGL}\cdot[\mathrm{D6PGluconoLactone}]}{\mathrm{Km6PGL}+[\mathrm{D6PGluconoLactone}]} \tag{35}$$

Table 58: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vm6PGL	Vm6PGL		4.0	$\mathrm{mmol}\cdot\mathrm{l}^{-1}\cdot(60\,\mathrm{s})^{-1}$	☑
Km6PGL	Km6PGL		0.8	$\mathrm{mmol}\cdot\mathrm{l}^{-1}$	☑

7.18 Reaction vGluDH

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

Name vGluDH

SBO:0000200 redox reaction

Reaction equation

$$\mathrm{D6PGluconate} + \mathrm{NADP} \xrightarrow{\mathrm{NADPH}} \mathrm{Ribulose5P} + \mathrm{NADPH} \tag{36}$$

Reactants

Table 59: Properties of each reactant.

Id	Name	SBO
D6PGluconate	6-phosphogluconate	
NADP	NADP+	

Modifier

Table 60: Properties of each modifier.

Id	Name	SBO
NADPH	NADPH	

Products

Table 61: Properties of each product.

Id	Name	SBO
Ribulose5P	ribulose 5-phosphate	
NADPH	NADPH	

Kinetic Law

Derived unit contains undeclared units

$$v_{18} = \mathrm{vol}\,(\mathrm{cytoplasm}) \cdot \frac{\frac{\mathrm{VmGluDH} \cdot [\mathrm{D6PGluconate}] \cdot [\mathrm{NADP}]}{\mathrm{KmGluconate} \cdot \mathrm{KmNADP}}}{\left(1 + \frac{[\mathrm{D6PGluconate}]}{\mathrm{KmGluconate}} + \frac{[\mathrm{NADPH}]}{\mathrm{KiNADPH}}\right) \cdot \left(1 + \frac{[\mathrm{NADP}]}{\mathrm{KmNADP}}\right)} \tag{37}$$

Table 62: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
VmGluDH	VmGluDH		4.00	$\mathrm{mmol} \cdot \mathrm{l}^{-1} \cdot (60\ \mathrm{s})^{-1}$	☑
KmGluconate	KmGluconate		0.02	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KmNADP	KmNADP		0.03	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KiNADPH	KiNADPH		0.03	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑

7.19 Reaction vPPI

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

Name vPPI

SBO:0000377 isomerisation

Reaction equation

$$\text{Ribulose5P} \rightleftharpoons \text{Ribose5P} \tag{38}$$

Reactant

Table 63: Properties of each reactant.

Id	Name	SBO
Ribulose5P	ribulose 5-phosphate	

Product

Table 64: Properties of each product.

Id	Name	SBO
Ribose5P	ribose 5-phosphate	

Kinetic Law

Derived unit contains undeclared units

$$v_{19} = \text{vol}\,(\text{cytoplasm}) \cdot \frac{\frac{\text{VmPPIf} \cdot [\text{Ribulose5P}]}{\text{KmRibu5P}} - \frac{\text{VmPPIr} \cdot [\text{Ribose5P}]}{\text{KmRibo5P}}}{1 + \frac{[\text{Ribulose5P}]}{\text{KmRibu5P}} + \frac{[\text{Ribose5P}]}{\text{KmRibo5P}}} \tag{39}$$

Table 65: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
VmPPIf	VmPPIf		3458.0	$\text{mmol} \cdot \text{l}^{-1} \cdot (60\ \text{s})^{-1}$	☑
VmPPIr	VmPPIr		3458.0	$\text{mmol} \cdot \text{l}^{-1} \cdot (60\ \text{s})^{-1}$	☑
KmRibu5P	KmRibu5P		1.6	$\text{mmol} \cdot \text{l}^{-1}$	☑
KmRibo5P	KmRibo5P		1.6	$\text{mmol} \cdot \text{l}^{-1}$	☑

7.20 Reaction vTransk1

This is a reversible reaction of two reactants forming two products.

Name vTransk1

SBO:0000182 conversion

Reaction equation

$$\text{Ribose5P} + \text{Xyl5P} \rightleftharpoons \text{GA3P} + \text{Seduhept7P} \tag{40}$$

Reactants

Table 66: Properties of each reactant.

Id	Name	SBO
Ribose5P	ribose 5-phosphate	
Xyl5P	xylulose 5-phosphate	

Products

Table 67: Properties of each product.

Id	Name	SBO
GA3P	glyceraldehyde 3-phosphate	
Seduhept7P	sedoheptulose 7-phosphate	

Kinetic Law

Derived unit contains undeclared units

$$v_{20} = \text{vol}\,(\text{cytoplasm}) \cdot \frac{\frac{\text{VmTransk1f}\cdot[\text{Ribose5P}]\cdot[\text{Xyl5P}]}{\text{KmRibose5P}\cdot\text{KmXyl5P}} - \frac{\text{VmTransk1r}\cdot[\text{GA3P}]\cdot[\text{Seduhept7P}]}{\text{KmGA3P}\cdot\text{KmSeduhept}}}{\left(1 + \frac{[\text{Ribose5P}]}{\text{KmRibose5P}} + \frac{[\text{GA3P}]}{\text{KmGA3P}}\right)\cdot\left(1 + \frac{[\text{Xyl5P}]}{\text{KmXyl5P}} + \frac{[\text{Seduhept7P}]}{\text{KmSeduhept}}\right)} \tag{41}$$

Table 68: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
VmTransk1f	VmTransk1f		4.00	$\text{mmol} \cdot \text{l}^{-1} \cdot (60\ \text{s})^{-1}$	☑
VmTransk1r	VmTransk1r		2.00	$\text{mmol} \cdot \text{l}^{-1} \cdot (60\ \text{s})^{-1}$	☑

Id	Name	SBO	Value	Unit	Constant
KmRibose5P	KmRibose5P		0.10	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KmXyl5P	KmXyl5P		0.15	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KmGA3P	KmGA3P		0.10	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KmSeduhept	KmSeduhept		0.15	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑

7.21 Reaction vR5PI

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

Name vR5PI

SBO:0000377 isomerisation

Reaction equation

$$\mathrm{Ribulose5P} \rightleftharpoons \mathrm{Xyl5P} \tag{42}$$

Reactant

Table 69: Properties of each reactant.

Id	Name	SBO
Ribulose5P	ribulose 5-phosphate	

Product

Table 70: Properties of each product.

Id	Name	SBO
Xyl5P	xylulose 5-phosphate	

Kinetic Law

Derived unit contains undeclared units

$$v_{21} = \mathrm{vol}\,(\mathrm{cytoplasm}) \cdot \frac{\frac{\mathrm{VmR5PIf} \cdot [\mathrm{Ribulose5P}]}{\mathrm{KmRibu5P}} - \frac{\mathrm{VmR5PIr} \cdot [\mathrm{Xyl5P}]}{\mathrm{KmXyl}}}{1 + \frac{[\mathrm{Ribulose5P}]}{\mathrm{KmRibu5P}} + \frac{[\mathrm{Xyl5P}]}{\mathrm{KmXyl}}} \tag{43}$$

Table 71: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
VmR5PIf	VmR5PIf		1039.0	$\text{mmol} \cdot \text{l}^{-1} \cdot (60\ \text{s})^{-1}$	☑
VmR5PIr	VmR5PIr		1039.0	$\text{mmol} \cdot \text{l}^{-1} \cdot (60\ \text{s})^{-1}$	☑
KmRibu5P	KmRibu5P		1.5	$\text{mmol} \cdot \text{l}^{-1}$	☑
KmXyl	KmXyl		1.5	$\text{mmol} \cdot \text{l}^{-1}$	☑

7.22 Reaction vTransald

This is a reversible reaction of two reactants forming two products.

Name vTransald

SBO:0000182 conversion

Reaction equation

$$\text{Seduhept7P} + \text{GA3P} \rightleftharpoons \text{F6P} + \text{Erythrose4P} \tag{44}$$

Reactants

Table 72: Properties of each reactant.

Id	Name	SBO
Seduhept7P	sedoheptulose 7-phosphate	
GA3P	glyceraldehyde 3-phosphate	

Products

Table 73: Properties of each product.

Id	Name	SBO
F6P	Fructose 6 Phosphate	
Erythrose4P	erythrose 4-phosphate	

Kinetic Law

Derived unit contains undeclared units

$$v_{22} = \mathrm{vol}\,(\mathrm{cytoplasm}) \cdot \frac{\frac{\mathrm{VmTransaldf}\cdot[\mathrm{GA3P}]\cdot[\mathrm{Seduhept7P}]}{\mathrm{KmGA3P}\cdot\mathrm{KmSeduhept}} - \frac{\mathrm{VmTransaldr}\cdot[\mathrm{F6P}]\cdot[\mathrm{Erythrose4P}]}{\mathrm{KmF6P}\cdot\mathrm{KmEry4P}}}{\left(1+\frac{[\mathrm{GA3P}]}{\mathrm{KmGA3P}}+\frac{[\mathrm{F6P}]}{\mathrm{KmF6P}}\right)\cdot\left(1+\frac{[\mathrm{Seduhept7P}]}{\mathrm{KmSeduhept}}+\frac{[\mathrm{Erythrose4P}]}{\mathrm{KmEry4P}}\right)} \tag{45}$$

Table 74: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
VmTransaldf	VmTransaldf		55.000	$\mathrm{mmol}\cdot\mathrm{l}^{-1}\cdot(60\ \mathrm{s})^{-1}$	☑
VmTransaldr	VmTransaldr		10.000	$\mathrm{mmol}\cdot\mathrm{l}^{-1}\cdot(60\ \mathrm{s})^{-1}$	☑
KmGA3P	KmGA3P		0.220	$\mathrm{mmol}\cdot\mathrm{l}^{-1}$	☑
KmSeduhept	KmSeduhept		0.180	$\mathrm{mmol}\cdot\mathrm{l}^{-1}$	☑
KmF6P	KmF6P		0.320	$\mathrm{mmol}\cdot\mathrm{l}^{-1}$	☑
KmEry4P	KmEry4P		0.018	$\mathrm{mmol}\cdot\mathrm{l}^{-1}$	☑

7.23 Reaction vTransk2

This is a reversible reaction of two reactants forming two products.

Name vTransk2

SBO:0000182 conversion

Reaction equation

$$\mathrm{Xyl5P} + \mathrm{Erythrose4P} \rightleftharpoons \mathrm{GA3P} + \mathrm{F6P} \tag{46}$$

Reactants

Table 75: Properties of each reactant.

Id	Name	SBO
Xyl5P	xylulose 5-phosphate	
Erythrose4P	erythrose 4-phosphate	

Products

Table 76: Properties of each product.

Id	Name	SBO
GA3P	glyceraldehyde 3-phosphate	

Id	Name	SBO
F6P	Fructose 6 Phosphate	

Kinetic Law

Derived unit contains undeclared units

$$v_{23} = \mathrm{vol}\,(\mathrm{cytoplasm}) \cdot \frac{\frac{\mathrm{VmTransk2f}\cdot[\mathrm{Erythrose4P}]\cdot[\mathrm{Xyl5P}]}{\mathrm{KmEry4P}\cdot\mathrm{KmXyl5P}} - \frac{\mathrm{VmTransk2r}\cdot[\mathrm{F6P}]\cdot[\mathrm{GA3P}]}{\mathrm{KmF6P}\cdot\mathrm{KmGA3P}}}{\left(1 + \frac{[\mathrm{Xyl5P}]}{\mathrm{KmXyl5P}} + \frac{[\mathrm{GA3P}]}{\mathrm{KmGA3P}}\right)\cdot\left(1 + \frac{[\mathrm{Erythrose4P}]}{\mathrm{KmEry4P}} + \frac{[\mathrm{F6P}]}{\mathrm{KmF6P}}\right)} \tag{47}$$

Table 77: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
VmTransk2f	VmTransk2F		3.20	$\mathrm{mmol}\cdot\mathrm{l}^{-1}\cdot(60\ \mathrm{s})^{-1}$	☑
VmTransk2r	VmTransk2r		43.00	$\mathrm{mmol}\cdot\mathrm{l}^{-1}\cdot(60\ \mathrm{s})^{-1}$	☑
KmXyl5P	KmXyl5P		0.16	$\mathrm{mmol}\cdot\mathrm{l}^{-1}$	☑
KmEry4P	KmEry4P		0.09	$\mathrm{mmol}\cdot\mathrm{l}^{-1}$	☑
KmF6P	KmF6P		1.10	$\mathrm{mmol}\cdot\mathrm{l}^{-1}$	☑
KmGA3P	KmGA3P		2.10	$\mathrm{mmol}\cdot\mathrm{l}^{-1}$	☑

7.24 Reaction vNADPH

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

Name vNADPH

SBO:0000201 oxidation

Reaction equation

$$\mathrm{NADPH} \longrightarrow \mathrm{NADP} \tag{48}$$

Reactant

Table 78: Properties of each reactant.

Id	Name	SBO
NADPH	NADPH	

Product

Table 79: Properties of each product.

Id	Name	SBO
NADP	NADP+	

Kinetic Law

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

$$v_{24} = \mathrm{vol}\,(\mathrm{cytoplasm}) \cdot \mathrm{kNADPH} \cdot [\mathrm{NADPH}] \tag{49}$$

Table 80: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
kNADPH	kNADPH		2.0	$(60\ \mathrm{s})^{-1}$	☑

7.25 Reaction vGLT

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

Name Glucose transport

SBO:0000185 transport reaction

Reaction equation

$$\mathrm{GLCo} \rightleftharpoons \mathrm{GLCi} \tag{50}$$

Reactant

Table 81: Properties of each reactant.

Id	Name	SBO
GLCo	Extracellular Glucose	

Product

Table 82: Properties of each product.

Id	Name	SBO
GLCi	Glucose in Cytosol	

Kinetic Law

Derived unit contains undeclared units

$$v_{25} = \mathrm{vol}\,(\mathrm{cytoplasm}) \cdot \frac{\mathrm{VmGLT} \cdot \left([\mathrm{GLCo}] - \frac{[\mathrm{GLCi}]}{\mathrm{KeqGLT}}\right)}{\mathrm{KmGLTGLCo} \cdot \left(1 + \frac{[\mathrm{GLCo}]}{\mathrm{KmGLTGLCo}} + \frac{[\mathrm{GLCi}]}{\mathrm{KmGLTGLCi}} + \frac{0.91 \cdot [\mathrm{GLCo}] \cdot [\mathrm{GLCi}]}{\mathrm{KmGLTGLCi} \cdot \mathrm{KmGLTGLCo}}\right)} \tag{51}$$

Table 83: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
VmGLT	VmGLT		97.264	$\mathrm{mmol} \cdot \mathrm{l}^{-1} \cdot (60\ \mathrm{s})^{-1}$	☑
KeqGLT	KeqGLT		1.000	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KmGLTGLCo	KmGLTGLCo		1.192	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KmGLTGLCi	KmGLTGLCi		1.192	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑

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 P

Name High energy phosphates

SBO:0000247 simple chemical

Initial concentration $5\ \mathrm{mmol} \cdot \mathrm{l}^{-1}$

This species takes part in five reactions (as a reactant in vGLK, vPFK, vATP and as a product in vPGK, vPYK).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{P} = v_7 + v_{10} - v_1 - v_3 - v_{14} \tag{52}$$

8.2 Species G6P

Name Glucose 6 Phosphate

SBO:0000247 simple chemical

Initial concentration $1.39\ \mathrm{mmol} \cdot \mathrm{l}^{-1}$

This species takes part in three reactions (as a reactant in vPGI, vG6PDH and as a product in vGLK).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{G6P} = v_1 - v_2 - v_{16} \tag{53}$$

8.3 Species F6P

Name Fructose 6 Phosphate

SBO:0000247 simple chemical

Initial concentration $0.28\ \mathrm{mmol} \cdot \mathrm{l}^{-1}$

This species takes part in four reactions (as a reactant in vPFK and as a product in vPGI, vTransald, vTransk2).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{F6P} = v_2 + v_{22} + v_{23} - v_3 \tag{54}$$

8.4 Species F16P

Name Fructose-1,6 bisphosphate

SBO:0000247 simple chemical

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

This species takes part in two reactions (as a reactant in vALD and as a product in vPFK).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{F16P} = v_3 - v_4 \tag{55}$$

8.5 Species NADH

Name NADH

SBO:0000247 simple chemical

Initial concentration $0.39\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in four reactions (as a reactant in vG3PDH, vADH and as a product in vGAPDH, vSUC).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{NADH} = v_6 + 3v_{12} - v_5 - v_{13} \tag{56}$$

8.6 Species NAD

Name NAD

SBO:0000247 simple chemical

Initial concentration $1.2\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in four reactions (as a reactant in vGAPDH, vSUC and as a product in vG3PDH, vADH).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{NAD} = v_5 + v_{13} - v_6 - 3v_{12} \tag{57}$$

8.7 Species BPG

Name 1,3-bisphosphoglycerate

SBO:0000247 simple chemical

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

This species takes part in two reactions (as a reactant in vPGK and as a product in vGAPDH).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{BPG} = v_6 - v_7 \tag{58}$$

8.8 Species P3G

Name 3-phosphoglycerate

SBO:0000247 simple chemical

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

This species takes part in two reactions (as a reactant in vPGM and as a product in vPGK).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{P3G} = v_7 - v_8 \tag{59}$$

8.9 Species P2G

Name 2-phosphoglycerate

SBO:0000247 simple chemical

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

This species takes part in two reactions (as a reactant in vENO and as a product in vPGM).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{P2G} = v_8 - v_9 \tag{60}$$

8.10 Species PEP

Name Phosphoenolpyruvate

SBO:0000247 simple chemical

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

This species takes part in two reactions (as a reactant in vPYK and as a product in vENO).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{PEP} = v_9 - v_{10} \tag{61}$$

8.11 Species PYR

Name Pyruvate

SBO:0000247 simple chemical

Initial concentration $3.36\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in vPDC and as a product in vPYK).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{PYR} = v_{10} - v_{11} \tag{62}$$

8.12 Species ACE

Name Acetaldehyde

SBO:0000247 simple chemical

Initial concentration $0.04\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in three reactions (as a reactant in vSUC, vADH and as a product in vPDC).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ACE} = v_{11} - 2v_{12} - v_{13} \tag{63}$$

8.13 Species CO2

Name CO2

SBO:0000247 simple chemical

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{CO2} = 0 \tag{64}$$

8.14 Species ETOH

Name Ethanol

SBO:0000247 simple chemical

Initial concentration $50\ \mathrm{mmol} \cdot \mathrm{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ETOH} = 0 \tag{65}$$

8.15 Species SUCC

Name Succinate

SBO:0000247 simple chemical

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{SUCC} = 0 \tag{66}$$

8.16 Species X

Name X

SBO:0000291 empty set

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{X} = 0 \tag{67}$$

8.17 Species GA3P

Name glyceraldehyde 3-phosphate

SBO:0000247 simple chemical

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

This species takes part in six reactions (as a reactant in vGAPDH, vTPI, vTransald and as a product in vALD, vTransk1, vTransk2).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{GA3P} = v_4 + v_{20} + v_{23} - v_6 - v_{15} - v_{22} \tag{68}$$

8.18 Species DHAP

Name dihydroxyacetone phosphate

SBO:0000247 simple chemical

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

This species takes part in three reactions (as a reactant in vG3PDH and as a product in vALD, vTPI).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{DHAP} = v_4 + v_{15} - v_5 \tag{69}$$

8.19 Species GLY

Name Glycerol

SBO:0000247 simple chemical

Initial concentration $0.15\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in one reaction (as a product in vG3PDH), which does not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{GLY} = 0 \tag{70}$$

8.20 Species D6PGluconoLactone

Name D-6-phosphoglucono-delta-lactone

SBO:0000247 simple chemical

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

This species takes part in two reactions (as a reactant in v6PGL and as a product in vG6PDH).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{D6PGluconoLactone} = v_{16} - v_{17} \tag{71}$$

8.21 Species D6PGluconate

Name 6-phosphogluconate

SBO:0000247 simple chemical

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

This species takes part in two reactions (as a reactant in vGluDH and as a product in v6PGL).

$$\frac{\text{d}}{\text{d}t}\text{D6PGluconate} = v_{17} - v_{18} \tag{72}$$

8.22 Species NADP

Name NADP+

SBO:0000247 simple chemical

Initial concentration $0.4\ \text{mmol} \cdot \text{l}^{-1}$

This species takes part in three reactions (as a reactant in vG6PDH, vGluDH and as a product in vNADPH).

$$\frac{\text{d}}{\text{d}t}\text{NADP} = v_{24} - v_{16} - v_{18} \tag{73}$$

8.23 Species NADPH

Name NADPH

SBO:0000247 simple chemical

Initial concentration $1.6\ \text{mmol} \cdot \text{l}^{-1}$

This species takes part in five reactions (as a reactant in vNADPH and as a product in vG6PDH, vGluDH and as a modifier in vG6PDH, vGluDH).

$$\frac{\text{d}}{\text{d}t}\text{NADPH} = v_{16} + v_{18} - v_{24} \tag{74}$$

8.24 Species Ribulose5P

Name ribulose 5-phosphate

SBO:0000247 simple chemical

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

This species takes part in three reactions (as a reactant in vPPI, vR5PI and as a product in vGluDH).

$$\frac{\text{d}}{\text{d}t}\text{Ribulose5P} = v_{18} - v_{19} - v_{21} \tag{75}$$

8.25 Species Ribose5P

Name ribose 5-phosphate

SBO:0000247 simple chemical

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

This species takes part in two reactions (as a reactant in vTransk1 and as a product in vPPI).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Ribose5P} = v_{19} - v_{20} \tag{76}$$

8.26 Species Xyl5P

Name xylulose 5-phosphate

SBO:0000247 simple chemical

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

This species takes part in three reactions (as a reactant in vTransk1, vTransk2 and as a product in vR5PI).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Xyl5P} = v_{21} - v_{20} - v_{23} \tag{77}$$

8.27 Species Seduhept7P

Name sedoheptulose 7-phosphate

SBO:0000247 simple chemical

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

This species takes part in two reactions (as a reactant in vTransald and as a product in vTransk1).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Seduhept7P} = v_{20} - v_{22} \tag{78}$$

8.28 Species Erythrose4P

Name erythrose 4-phosphate

SBO:0000247 simple chemical

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

This species takes part in two reactions (as a reactant in vTransk2 and as a product in vTransald).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Erythrose4P} = v_{22} - v_{23} \tag{79}$$

8.29 Species GLCo

Name Extracellular Glucose

SBO:0000247 simple chemical

Initial concentration $50\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{GLCo} = 0 \tag{80}$$

8.30 Species GLCi

Name Glucose in Cytosol

SBO:0000247 simple chemical

Initial concentration $0.087\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in vGLK and as a product in vGLT).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{GLCi} = v_{25} - v_1 \tag{81}$$

8.31 Species F26BP

Name F2,6P

SBO:0000247 simple chemical

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{F26BP} = 0 \tag{82}$$

A Glossary of Systems Biology Ontology Terms

SBO:0000182 conversion: Biochemical reaction that results in the modification of some covalent bonds

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

SBO:0000200 redox reaction: Chemical process in which atoms have their oxidation number (oxidation state) changed

SBO:0000201 oxidation: Chemical process during which a molecular entity loses electrons

SBO:0000205 composite biochemical process: Process that involves the participation of chemical or biological entities and is composed of several elementary steps or reactions.

SBO:0000211 removal of a chemical group: Covalent reaction that results in the removal of a chemical group from a molecule

SBO:0000216 phosphorylation: Addition of a phosphate group (-H2PO4) to a chemical entity

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

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:0000291 empty set: Entity defined by the absence of any actual object. An empty set is often used to represent the source of a creation process or the result of a degradation process.

SBO:0000376 hydrolysis: Decomposition of a compound by reaction with water, where the hydroxyl and H groups are incorporated into different product

SBO:0000377 isomerisation: A reaction in which the principal reactant and principal product are isomers of each othe

SBO:0000399 decarboxylation: A process in which a carboxyl group (COOH) is removed from a molecule as carbon dioxide

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