SBML Model Report

Model name: "Conant2007_glycolysis_2C"

May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 1 format. This model was created by the following three authors: Gavin Conant[1], Lukas Endler[2] and Kenneth Wolfe[3] at September twelveth 2007 at 8:25 a. m. and last time modified at May 16th 2012 at 2:27 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	28
events	0	constraints	0
reactions	21	function definitions	0
global parameters	2	unit definitions	8
rules	0	initial assignments	0

Model Notes

This a model from the article:
Increased glycolytic flux as an outcome of whole-genome duplication in yeast.
Conant GC, Wolfe KH Mol. Syst. Biol. [2007 ; Volume: 3 (Issue:)]: 129 17667951 ,
Abstract:
After whole-genome duplication (WGD), deletions return most loci to single copy. However,

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duplicate loci may survive through selection for increased dosage. Here, we show how the WGD increased copy number of some glycolytic genes could have conferred an almost immediate selective advantage to an ancestor of Saccharomyces cerevisiae, providing a rationale for the success of the WGD. We propose that the loss of other redundant genes throughout the genome resulted in incremental dosage increases for the surviving duplicated glycolytic genes. This increase gave post-WGD yeasts a growth advantage through rapid glucose fermentation; one of this lineage's many adaptations to glucose-rich environments. Our hypothesis is supported by data from enzyme kinetics and comparative genomics. Because changes in gene dosage follow directly from post-WGD deletions, dosage selection can confer an almost instantaneous benefit after WGD, unlike neofunctionalization or subfunctionalization, which require specific mutations. We also show theoretically that increased fermentative capacity is of greatest advantage when glucose resources are both large and dense, an observation potentially related to the appearance of angiosperms around the time of WGD.

This model reproduces fig. 2C from the corrigendum to the publication
The parameter **Vmax_PDH** was corrected by a factor 60 from 6.32 mM/min in the publication to 379.2 mM/min in accordance with the authors.
see the corrigendum at msb or its pubmed entry (pmid:18594520)

This model comprises the glycolysis model from Pritchard and Kell (2002) with an extension for the metabolisation of pyruvate in the mitochondria by pyruvate dehydrogenase and an additional parameter, **WGD_E** , to adjust for the differing enzyme concentrations before the whole genome duplication (WGD).
To switch off transport of pyruvate to the mitochondria, set the parameter **t_m** = 0.
Figure 2C from the article can be reproduced by manually changing the value of parameter **WGD_E** in the range between 0.65 and 1.0 and calculating the ratios of ratio of **PDC/PDH** fluxes in the altered model to the one of the model with **WGD_E** = 1.

2 Unit Definitions

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

2.1 Unit `time`

Name minute

Definition $60\ \mathrm{s}$

2.2 Unit `substance`

Name mmol

Definition mmol

2.3 Unit `mM`

Name mM

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

2.4 Unit `mmpmin`

Name mmolepermin

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

2.5 Unit `mMpmin`

Name mMpermin

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

2.6 Unit `pmin`

Name permin

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

2.7 Unit `lpmin`

Name permin

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

2.8 Unit `pmMpmin`

Name permMpermin

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

2.9 Unit `volume`

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

Definition l

2.10 Unit area

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

Definition m^2

2.11 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
cyto	cytoplasm		3	1	litre	☑	
mito	mitochondrion		3	1	litre	☑	

3.1 Compartment cyto

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

Name cytoplasm

3.2 Compartment mito

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

Name mitochondrion

4 Species

This model contains 28 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 7 provides further details and the derived rates of change of each species.

Table 3: Properties of each species.

Id	Name	Compartment	Derived Unit	Constant	Boundary Condition
GLCi		cyto	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
ATP		cyto	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
G6P		cyto	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
ADP		cyto	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
F6P		cyto	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
F16bP		cyto	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
F26bP	Fru2,6-P2	cyto	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	☑
AMP		cyto	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
DHAP		cyto	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
GAP		cyto	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
NAD		cyto	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
BPG		cyto	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
NADH		cyto	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
P3G		cyto	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
P2G		cyto	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
PEP		cyto	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
PYR		cyto	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
PYRmito		mito	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
AcAld		cyto	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
GLCo		cyto	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	☑
CO2		cyto	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	☑

Id	Name	Compartment	Derived Unit	Constant	Boundary Condition
EtOH		cyto	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	☑
Glycerol		cyto	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	☑
Glycogen		cyto	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	☑
Trehalose		cyto	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	☑
Succinate		cyto	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	☑
AcCoA		mito	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	☑
CO2mito		mito	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	☑

5 Parameters

This model contains two global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
t_m	toggle_transport		1.00	dimensionless	☑
WGD_E	WGD enzyme conc change		0.65	dimensionless	☑

6 Reactions

This model contains 21 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	HXT	HXT	$\mathrm{GLCo} \rightleftharpoons \mathrm{GLCi}$	
2	HXK	HXK	$\mathrm{GLCi} + \mathrm{ATP} \rightleftharpoons \mathrm{G6P} + \mathrm{ADP}$	
3	PGI	PGI	$\mathrm{G6P} \rightleftharpoons \mathrm{F6P}$	
4	PFK	PFK	$\mathrm{ATP} + \mathrm{F6P} \xrightarrow{\mathrm{AMP,\ F26bP}} \mathrm{ADP} + \mathrm{F16bP}$	
5	FBA	FBA	$\mathrm{F16bP} \rightleftharpoons \mathrm{DHAP} + \mathrm{GAP}$	
6	TPI	TPI	$\mathrm{DHAP} \rightleftharpoons \mathrm{GAP}$	
7	TDH	TDH	$\mathrm{GAP} + \mathrm{NAD} \rightleftharpoons \mathrm{BPG} + \mathrm{NADH}$	
8	PGK	PGK	$\mathrm{ADP} + \mathrm{BPG} \rightleftharpoons \mathrm{ATP} + \mathrm{P3G}$	
9	PGM	PGM	$\mathrm{P3G} \rightleftharpoons \mathrm{P2G}$	
10	ENO	ENO	$\mathrm{P2G} \rightleftharpoons \mathrm{PEP}$	
11	PYK	PYK	$\mathrm{ADP} + \mathrm{PEP} \rightleftharpoons \mathrm{ATP} + \mathrm{PYR}$	
12	PDC	PDC	$\mathrm{PYR} \longrightarrow \mathrm{AcAld} + \mathrm{CO2}$	
13	ADH	ADH	$\mathrm{NAD} + \mathrm{EtOH} \rightleftharpoons \mathrm{NADH} + \mathrm{AcAld}$	
14	ATPase		$\mathrm{ATP} \longrightarrow \mathrm{ADP}$	
15	AK	adenylate_kinase	$2\,\mathrm{ADP} \rightleftharpoons \mathrm{ATP} + \mathrm{AMP}$	
16	G3PDH	glycerol-3-phosphate_dehydrogenase	$\mathrm{DHAP} + \mathrm{NADH} \rightleftharpoons \mathrm{NAD} + \mathrm{Glycerol}$	
17	glycogen_branch	glycogenbranch	$\mathrm{ATP} + \mathrm{G6P} \longrightarrow \mathrm{ADP} + \mathrm{Glycogen}$	
18	trehalose_synth	trehalose_synthesis	$\mathrm{ATP} + 2\,\mathrm{G6P} \longrightarrow \mathrm{ADP} + \mathrm{Trehalose}$	
19	succinate_syn	succinate_synthesis	$3\,\mathrm{NAD} + 2\,\mathrm{AcAld} \longrightarrow 3\,\mathrm{NADH} + \mathrm{Succinate}$	
20	PYR_shut	pyruvate_shuttling	$\mathrm{PYR} \rightleftharpoons \mathrm{PYRmito}$	
21	PDH	pyruvate dehydrogenase	$\mathrm{PYRmito} \xrightarrow{\mathrm{NAD,\ NADH}} \mathrm{AcCoA} + \mathrm{CO2mito}$	

6.1 Reaction HXT

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

Name HXT

Reaction equation

$$\mathrm{GLCo} \rightleftharpoons \mathrm{GLCi} \tag{1}$$

Reactant

Table 6: Properties of each reactant.

Id	Name	SBO
GLCo		

Product

Table 7: Properties of each product.

Id	Name	SBO
GLCi		

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \frac{\frac{\mathrm{Vmax\_1} \cdot \mathrm{WGD\_E} \cdot (\mathrm{[GLCo]} - \mathrm{[GLCi]})}{\mathrm{Kglc\_1}}}{1 + \frac{\mathrm{[GLCo]} + \mathrm{[GLCi]}}{\mathrm{Kglc\_1}} + \frac{\mathrm{Ki\_1} \cdot \mathrm{[GLCo]} \cdot \mathrm{[GLCi]}}{\mathrm{Kglc\_1}^2}} \tag{2}$$

Table 8: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax_1			97.240	$\mathrm{mmol} \cdot (60\ \mathrm{s})^{-1}$	☑
Kglc_1			1.192	$\mathrm{l}^{-1} \cdot \mathrm{mmol}$	☑
Ki_1			0.910	dimensionless	☑

6.2 Reaction HXK

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

Name HXK

Reaction equation

$$\mathrm{GLCi} + \mathrm{ATP} \rightleftharpoons \mathrm{G6P} + \mathrm{ADP} \tag{3}$$

Reactants

Table 9: Properties of each reactant.

Id	Name	SBO
GLCi		
ATP		

Products

Table 10: Properties of each product.

Id	Name	SBO
G6P		
ADP		

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \frac{\mathrm{vol}\,(\mathrm{cyto}) \cdot \mathrm{WGD\_E} \cdot \mathrm{Vmax\_2} \cdot \left(\frac{[\mathrm{GLCi}] \cdot [\mathrm{ATP}]}{\mathrm{Kglc\_2} \cdot \mathrm{Katp\_2}} - \frac{[\mathrm{G6P}] \cdot [\mathrm{ADP}]}{\mathrm{Kglc\_2} \cdot \mathrm{Katp\_2} \cdot \mathrm{Keq\_2}} \right)}{\left(1 + \frac{[\mathrm{GLCi}]}{\mathrm{Kglc\_2}} + \frac{[\mathrm{G6P}]}{\mathrm{Kg6p\_2}}\right) \cdot \left(1 + \frac{[\mathrm{ATP}]}{\mathrm{Katp\_2}} + \frac{[\mathrm{ADP}]}{\mathrm{Kadp\_2}}\right)} \tag{4}$$

Table 11: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax_2			236.70	$\mathrm{mmol} \cdot (60\,\mathrm{s})^{-1} \cdot \mathrm{l}^{-1}$	☑
Kglc_2			0.08	$\mathrm{l}^{-1} \cdot \mathrm{mmol}$	☑
Katp_2			0.15	$\mathrm{l}^{-1} \cdot \mathrm{mmol}$	☑
Keq_2			2000.00	dimensionless	☑

Id	Name	SBO	Value	Unit	Constant
Kg6p_2			30.00	$l^{-1} \cdot mmol$	☑
Kadp_2			0.23	$l^{-1} \cdot mmol$	☑

6.3 Reaction PGI

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

Name PGI

Reaction equation

$$G6P \rightleftharpoons F6P \tag{5}$$

Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
G6P		

Product

Table 13: Properties of each product.

Id	Name	SBO
F6P		

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \frac{\mathrm{vol}\,(\mathrm{cyto}) \cdot \mathrm{Vmax\_3} \cdot \mathrm{WGD\_E} \cdot \left(\frac{[\mathrm{G6P}]}{\mathrm{Kg6p\_3}} - \frac{[\mathrm{F6P}]}{\mathrm{Kg6p\_3} \cdot \mathrm{Keq\_3}} \right)}{1 + \frac{[\mathrm{G6P}]}{\mathrm{Kg6p\_3}} + \frac{[\mathrm{F6P}]}{\mathrm{Kf6p\_3}}} \tag{6}$$

Table 14: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax_3			1056.00	$\mathrm{mmol} \cdot (60\,\mathrm{s})^{-1} \cdot l^{-1}$	☑

Id	Name	SBO	Value	Unit	Constant
Kg6p_3			1.40	$l^{-1} \cdot mmol$	☑
Keq_3			0.29	dimensionless	☑
Kf6p_3			0.30	$l^{-1} \cdot mmol$	☑

6.4 Reaction PFK

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

Name PFK

Reaction equation

$$\mathrm{ATP} + \mathrm{F6P} \xrightarrow{\text{AMP, F26bP}} \mathrm{ADP} + \mathrm{F16bP} \tag{7}$$

Reactants

Table 15: Properties of each reactant.

Id	Name	SBO
ATP		
F6P		

Modifiers

Table 16: Properties of each modifier.

Id	Name	SBO
AMP		
F26bP	Fru2,6-P2	

Products

Table 17: Properties of each product.

Id	Name	SBO
ADP		
F16bP		

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \mathrm{vol}\,(\mathrm{cyto}) \cdot \mathrm{Vmax\_4} \cdot \mathrm{WGD\_E} \cdot \frac{\mathrm{gR\_4} \cdot \frac{[\mathrm{F6P}]}{\mathrm{Kf6p\_4}} \cdot \frac{[\mathrm{ATP}]}{\mathrm{Katp\_4}} \cdot \left(1 + \frac{[\mathrm{F6P}]}{\mathrm{Kf6p\_4}} + \frac{[\mathrm{ATP}]}{\mathrm{Katp\_4}} + \frac{\frac{\mathrm{gR\_4} \cdot [\mathrm{F6P}]}{\mathrm{Kf6p\_4}} \cdot [\mathrm{ATP}]}{\mathrm{Katp\_4}}\right)}{\left(1 + \frac{[\mathrm{F6P}]}{\mathrm{Kf6p\_4}} + \frac{[\mathrm{ATP}]}{\mathrm{Katp\_4}} + \frac{\frac{\mathrm{gR\_4} \cdot [\mathrm{F6P}]}{\mathrm{Kf6p\_4}} \cdot [\mathrm{ATP}]}{\mathrm{Katp\_4}}\right)^2 + \mathrm{L0\_4} \cdot \left(\frac{1 + \frac{\mathrm{Ciatp\_4} \cdot [\mathrm{ATP}]}{\mathrm{Kiatp\_4}}}{1 + \frac{[\mathrm{ATP}]}{\mathrm{Kiatp\_4}}}\right)^2 \cdot \left(\frac{1 + \frac{\mathrm{Camp\_4} \cdot [\mathrm{AMP}]}{\mathrm{Kamp\_4}}}{1 + \frac{[\mathrm{AMP}]}{\mathrm{Kamp\_4}}}\right)^2 \cdot \left(\frac{1 + \frac{\mathrm{Cf26\_4} \cdot [\mathrm{F26bP}]}{\mathrm{Kf26\_4}} + \frac{\mathrm{Cf16\_4} \cdot [\mathrm{F16bP}]}{\mathrm{Kf16\_4}}}{1 + \frac{[\mathrm{F26bP}]}{\mathrm{Kf26\_4}} + \frac{[\mathrm{F16bP}]}{\mathrm{Kf16\_4}}}\right)^2} \tag{8}$$

Table 18: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax_4			110.000	$\mathrm{mmol} \cdot (60\,\mathrm{s})^{-1} \cdot \mathrm{l}^{-1}$	☑
gR_4			5.120	dimensionless	☑
Kf6p_4			0.100	$\mathrm{l}^{-1} \cdot \mathrm{mmol}$	☑
Katp_4			0.710	$\mathrm{l}^{-1} \cdot \mathrm{mmol}$	☑
L0_4			0.660	dimensionless	☑
Ciatp_4			100.000	dimensionless	☑
Kiatp_4			0.650	$\mathrm{l}^{-1} \cdot \mathrm{mmol}$	☑
Camp_4			0.085	dimensionless	☑
Kamp_4			0.100	$\mathrm{l}^{-1} \cdot \mathrm{mmol}$	☑
Cf26_4			0.017	dimensionless	☑
Kf26_4			$6.82 \cdot 10^{-4}$	$\mathrm{l}^{-1} \cdot \mathrm{mmol}$	☑
Cf16_4			0.397	dimensionless	☑
Kf16_4			0.111	$\mathrm{l}^{-1} \cdot \mathrm{mmol}$	☑
Catp_4			3.000	dimensionless	☑

6.5 Reaction FBA

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

Name FBA

Reaction equation

$$\mathrm{F16bP} \rightleftharpoons \mathrm{DHAP} + \mathrm{GAP} \tag{9}$$

Reactant

Table 19: Properties of each reactant.

Id	Name	SBO
F16bP		

Products

Table 20: Properties of each product.

Id	Name	SBO
DHAP		
GAP		

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \frac{\mathrm{vol}\,(\mathrm{cyto}) \cdot \mathrm{Vmax\_5} \cdot \mathrm{WGD\_E} \cdot \left(\frac{[\mathrm{F16bP}]}{\mathrm{Kf16bp\_5}} - \frac{[\mathrm{DHAP}] \cdot [\mathrm{GAP}]}{\mathrm{Kf16bp\_5} \cdot \mathrm{Keq\_5}} \right)}{1 + \frac{[\mathrm{F16bP}]}{\mathrm{Kf16bp\_5}} + \frac{[\mathrm{DHAP}]}{\mathrm{Kdhap\_5}} + \frac{[\mathrm{GAP}]}{\mathrm{Kgap\_5}} + \frac{[\mathrm{F16bP}] \cdot [\mathrm{GAP}]}{\mathrm{Kf16bp\_5} \cdot \mathrm{Kigap\_5}} + \frac{[\mathrm{DHAP}] \cdot [\mathrm{GAP}]}{\mathrm{Kdhap\_5} \cdot \mathrm{Kgap\_5}}} \tag{10}$$

Table 21: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax_5			94.690	$\mathrm{mmol} \cdot (60\,\mathrm{s})^{-1} \cdot \mathrm{l}^{-1}$	☑
Kf16bp_5			0.300	$\mathrm{l}^{-1} \cdot \mathrm{mmol}$	☑
Keq_5			0.069	$\mathrm{l}^{-1} \cdot \mathrm{mmol}$	☑
Kdhap_5			2.000	$\mathrm{l}^{-1} \cdot \mathrm{mmol}$	☑
Kgap_5			2.400	$\mathrm{l}^{-1} \cdot \mathrm{mmol}$	☑
Kigap_5			10.000	$\mathrm{l}^{-1} \cdot \mathrm{mmol}$	☑

6.6 Reaction TPI

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

Name TPI

Reaction equation

$$\mathrm{DHAP} \rightleftharpoons \mathrm{GAP} \tag{11}$$

Reactant

Table 22: Properties of each reactant.

Id	Name	SBO
DHAP		

Product

Table 23: Properties of each product.

Id	Name	SBO
GAP		

Kinetic Law

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

$$v_6 = \mathrm{vol}\,(\mathrm{cyto}) \cdot (\mathrm{k1\_6} \cdot [\mathrm{DHAP}] - \mathrm{k2\_6} \cdot [\mathrm{GAP}]) \tag{12}$$

Table 24: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1_6			450000.000	$(60\ \mathrm{s})^{-1}$	☑
k2_6			10^7	$(60\ \mathrm{s})^{-1}$	☑

6.7 Reaction TDH

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

Name TDH

Reaction equation

$$\mathrm{GAP} + \mathrm{NAD} \rightleftharpoons \mathrm{BPG} + \mathrm{NADH} \tag{13}$$

Reactants

Table 25: Properties of each reactant.

Id	Name	SBO
GAP		
NAD		

Products

Table 26: Properties of each product.

Id	Name	SBO
BPG		
NADH		

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \frac{\mathrm{vol}\,(\mathrm{cyto}) \cdot \mathrm{C\_7} \cdot \left(\frac{\mathrm{Vmaxf\_7} \cdot \mathrm{WGD\_E} \cdot [\mathrm{GAP}] \cdot [\mathrm{NAD}]}{\mathrm{Kgap\_7} \cdot \mathrm{Knad\_7}} - \frac{\mathrm{Vmaxr\_7} \cdot \mathrm{WGD\_E} \cdot [\mathrm{BPG}] \cdot [\mathrm{NADH}]}{\mathrm{Kbpg\_7} \cdot \mathrm{Knadh\_7}} \right)}{\left(1 + \frac{[\mathrm{GAP}]}{\mathrm{Kgap\_7}} + \frac{[\mathrm{BPG}]}{\mathrm{Kbpg\_7}}\right) \cdot \left(1 + \frac{[\mathrm{NAD}]}{\mathrm{Knad\_7}} + \frac{[\mathrm{NADH}]}{\mathrm{Knadh\_7}}\right)} \tag{14}$$

Table 27: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
C_7			1.000	dimensionless	☑
Vmaxf_7			1152.000	$\mathrm{mmol} \cdot (60\,\mathrm{s})^{-1} \cdot \mathrm{l}^{-1}$	☑
Kgap_7			0.210	$\mathrm{l}^{-1} \cdot \mathrm{mmol}$	☑
Knad_7			0.090	$\mathrm{l}^{-1} \cdot \mathrm{mmol}$	☑
Vmaxr_7			6719.000	$\mathrm{mmol} \cdot (60\,\mathrm{s})^{-1} \cdot \mathrm{l}^{-1}$	☑
Kbpg_7			0.010	$\mathrm{l}^{-1} \cdot \mathrm{mmol}$	☑
Knadh_7			0.060	$\mathrm{l}^{-1} \cdot \mathrm{mmol}$	☑

6.8 Reaction PGK

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

Name PGK

Reaction equation

$$\mathrm{ADP} + \mathrm{BPG} \rightleftharpoons \mathrm{ATP} + \mathrm{P3G} \tag{15}$$

Reactants

Table 28: Properties of each reactant.

Id	Name	SBO
ADP		
BPG		

Products

Table 29: Properties of each product.

Id	Name	SBO
ATP		
P3G		

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \frac{\mathrm{vol}\,(\mathrm{cyto}) \cdot \mathrm{Vmax\_8} \cdot \mathrm{WGD\_E} \cdot \frac{\mathrm{Keq\_8} \cdot [\mathrm{BPG}] \cdot [\mathrm{ADP}] - [\mathrm{P3G}] \cdot [\mathrm{ATP}]}{\mathrm{Kp3g\_8} \cdot \mathrm{Katp\_8}}}{\left(1 + \frac{[\mathrm{BPG}]}{\mathrm{Kbpg\_8}} + \frac{[\mathrm{P3G}]}{\mathrm{Kp3g\_8}}\right) \cdot \left(1 + \frac{[\mathrm{ADP}]}{\mathrm{Kadp\_8}} + \frac{[\mathrm{ATP}]}{\mathrm{Katp\_8}}\right)} \tag{16}$$

Table 30: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax_8			1288.000	$\mathrm{mmol} \cdot (60\,\mathrm{s})^{-1} \cdot \mathrm{l}^{-1}$	☑
Keq_8			3200.000	dimensionless	☑
Kp3g_8			0.530	$\mathrm{l}^{-1} \cdot \mathrm{mmol}$	☑
Katp_8			0.300	$\mathrm{l}^{-1} \cdot \mathrm{mmol}$	☑
Kbpg_8			0.003	$\mathrm{l}^{-1} \cdot \mathrm{mmol}$	☑
Kadp_8			0.200	$\mathrm{l}^{-1} \cdot \mathrm{mmol}$	☑

6.9 Reaction PGM

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

Name PGM

Reaction equation

$$\mathrm{P3G} \rightleftharpoons \mathrm{P2G} \tag{17}$$

Reactant

Table 31: Properties of each reactant.

Id	Name	SBO
P3G		

Product

Table 32: Properties of each product.

Id	Name	SBO
P2G		

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \frac{\mathrm{vol}\,(\mathrm{cyto}) \cdot \mathrm{Vmax\_9} \cdot \mathrm{WGD\_E} \cdot \left(\frac{[\mathrm{P3G}]}{\mathrm{Kp3g\_9}} - \frac{[\mathrm{P2G}]}{\mathrm{Kp3g\_9} \cdot \mathrm{Keq\_9}} \right)}{1 + \frac{[\mathrm{P3G}]}{\mathrm{Kp3g\_9}} + \frac{[\mathrm{P2G}]}{\mathrm{Kp2g\_9}}} \tag{18}$$

Table 33: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax_9			2585.00	$\mathrm{mmol} \cdot (60\ \mathrm{s})^{-1} \cdot \mathrm{l}^{-1}$	☑
Kp3g_9			1.20	$\mathrm{l}^{-1} \cdot \mathrm{mmol}$	☑
Keq_9			0.19	dimensionless	☑
Kp2g_9			0.08	$\mathrm{l}^{-1} \cdot \mathrm{mmol}$	☑

6.10 Reaction ENO

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

Name ENO

Reaction equation

$$\mathrm{P2G} \rightleftharpoons \mathrm{PEP} \tag{19}$$

Reactant

Table 34: Properties of each reactant.

Id	Name	SBO
P2G		

Product

Table 35: Properties of each product.

Id	Name	SBO
PEP		

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = \frac{\mathrm{vol\,(cyto)} \cdot \mathrm{Vmax\_10} \cdot \mathrm{WGD\_E} \cdot \left(\frac{[\mathrm{P2G}]}{\mathrm{Kp2g\_10}} - \frac{[\mathrm{PEP}]}{\mathrm{Kp2g\_10} \cdot \mathrm{Keq\_10}} \right)}{1 + \frac{[\mathrm{P2G}]}{\mathrm{Kp2g\_10}} + \frac{[\mathrm{PEP}]}{\mathrm{Kpep\_10}}} \tag{20}$$

Table 36: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax_10			201.60	$\mathrm{mmol} \cdot (60\,\mathrm{s})^{-1} \cdot \mathrm{l}^{-1}$	☑
Kp2g_10			0.04	$\mathrm{l}^{-1} \cdot \mathrm{mmol}$	☑
Keq_10			6.70	dimensionless	☑
Kpep_10			0.50	$\mathrm{l}^{-1} \cdot \mathrm{mmol}$	☑

6.11 Reaction PYK

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

Name PYK

Reaction equation

$$\mathrm{ADP} + \mathrm{PEP} \rightleftharpoons \mathrm{ATP} + \mathrm{PYR} \tag{21}$$

Reactants

Table 37: Properties of each reactant.

Id	Name	SBO
ADP		
PEP		

Products

Table 38: Properties of each product.

Id	Name	SBO
ATP		
PYR		

Kinetic Law

Derived unit contains undeclared units

$$v_{11} = \frac{\mathrm{vol}\,(\mathrm{cyto}) \cdot \mathrm{Vmax\_11} \cdot \mathrm{WGD\_E} \cdot \left(\frac{[\mathrm{PEP}] \cdot [\mathrm{ADP}]}{\mathrm{Kpep\_11} \cdot \mathrm{Kadp\_11}} - \frac{[\mathrm{PYR}] \cdot [\mathrm{ATP}]}{\mathrm{Kpep\_11} \cdot \mathrm{Kadp\_11} \cdot \mathrm{Keq\_11}} \right)}{\left(1 + \frac{[\mathrm{PEP}]}{\mathrm{Kpep\_11}} + \frac{[\mathrm{PYR}]}{\mathrm{Kpyr\_11}}\right) \cdot \left(1 + \frac{[\mathrm{ADP}]}{\mathrm{Kadp\_11}} + \frac{[\mathrm{ATP}]}{\mathrm{Katp\_11}}\right)} \tag{22}$$

Table 39: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax_11			1000.00	$\mathrm{mmol} \cdot (60\,\mathrm{s})^{-1} \cdot \mathrm{l}^{-1}$	☑
Kpep_11			0.14	$\mathrm{l}^{-1} \cdot \mathrm{mmol}$	☑
Kadp_11			0.53	$\mathrm{l}^{-1} \cdot \mathrm{mmol}$	☑
Keq_11			6500.00	dimensionless	☑

Id	Name	SBO	Value	Unit	Constant
Kpyr_11			21.00	$l^{-1} \cdot mmol$	☑
Katp_11			1.50	$l^{-1} \cdot mmol$	☑

6.12 Reaction PDC

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

Name PDC

Reaction equation

$$PYR \longrightarrow AcAld + CO2 \tag{23}$$

Reactant

Table 40: Properties of each reactant.

Id	Name	SBO
PYR		

Products

Table 41: Properties of each product.

Id	Name	SBO
AcAld		
CO2		

Kinetic Law

Derived unit contains undeclared units

$$v_{12} = \frac{\text{vol}(\text{cyto}) \cdot \text{Vmax\_12} \cdot \text{WGD\_E} \cdot \left(\frac{[\text{PYR}]}{\text{Kpyr\_12}}\right)^{\text{nH\_12}}}{1 + \left(\frac{[\text{PYR}]}{\text{Kpyr\_12}}\right)^{\text{nH\_12}}} \tag{24}$$

Table 42: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax_12			857.80	mmol · $(60\,\mathrm{s})^{-1}$ · l^{-1}	☑
Kpyr_12			4.33	$\mathrm{l}^{-1} \cdot \mathrm{mmol}$	☑
nH_12			1.90	dimensionless	☑

6.13 Reaction ADH

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

Name ADH

Reaction equation

$$\mathrm{NAD} + \mathrm{EtOH} \rightleftharpoons \mathrm{NADH} + \mathrm{AcAld} \tag{25}$$

Reactants

Table 43: Properties of each reactant.

Id	Name	SBO
NAD		
EtOH		

Products

Table 44: Properties of each product.

Id	Name	SBO
NADH		
AcAld		

Kinetic Law

Derived unit contains undeclared units

$$v_{13} = \frac{\mathrm{vol}(\mathrm{cyto}) \cdot \mathrm{Vmax\_13} \cdot \mathrm{WGD\_E} \cdot \left(\frac{[\mathrm{EtOH}] \cdot [\mathrm{NAD}]}{\mathrm{Ketoh\_13} \cdot \mathrm{Kinad\_1}} \right.}{1 + \frac{[\mathrm{NAD}]}{\mathrm{Kinad\_13}} + \frac{[\mathrm{EtOH}] \cdot \mathrm{Knad\_13}}{\mathrm{Kinad\_13} \cdot \mathrm{Ketoh\_13}} + \frac{[\mathrm{AcAld}] \cdot \mathrm{Knadh\_13}}{\mathrm{Kinadh\_13} \cdot \mathrm{Kacald\_13}} + \frac{[\mathrm{NADH}]}{\mathrm{Kinadh\_13}} + \frac{[\mathrm{EtOH}] \cdot [\mathrm{NAD}]}{\mathrm{Kinad\_13} \cdot \mathrm{Ketoh\_13}} + \frac{[\mathrm{NAD}] \cdot [\mathrm{AcAld}] \cdot \mathrm{Knadh\_13}}{\mathrm{Kinad\_13} \cdot \mathrm{Kinadh\_13} \cdot \mathrm{Kacald\_13}} + \frac{[\mathrm{Et}}{\mathrm{Kinac}}} \tag{26}$$

Table 45: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax_13			209.500	mmol · $(60\,\mathrm{s})^{-1}$ · l^{-1}	☑
Ketoh_13			17.000	$\mathrm{l}^{-1} \cdot$ mmol	☑
Kinad_13			0.920	$\mathrm{l}^{-1} \cdot$ mmol	☑
Keq_13			$6.9 \cdot 10^{-5}$	dimensionless	☑
Knad_13			0.170	$\mathrm{l}^{-1} \cdot$ mmol	☑
Knadh_13			0.110	$\mathrm{l}^{-1} \cdot$ mmol	☑
Kinadh_13			0.031	$\mathrm{l}^{-1} \cdot$ mmol	☑
Kacald_13			1.110	$\mathrm{l}^{-1} \cdot$ mmol	☑
Kiacald_13			1.100	$\mathrm{l}^{-1} \cdot$ mmol	☑
Kietoh_13			90.000	$\mathrm{l}^{-1} \cdot$ mmol	☑

6.14 Reaction ATPase

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

Reaction equation

$$\mathrm{ATP} \longrightarrow \mathrm{ADP} \tag{27}$$

Reactant

Table 46: Properties of each reactant.

Id	Name	SBO
ATP		

Product

Table 47: Properties of each product.

Id	Name	SBO
ADP		

Kinetic Law

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

$$v_{14} = \mathrm{vol}\,(\mathrm{cyto}) \cdot \mathrm{Katpase\_14} \cdot [\mathrm{ATP}] \tag{28}$$

Table 48: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Katpase_14			39.5	$(60\ \mathrm{s})^{-1}$	☑

6.15 Reaction AK

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

Name adenylate_kinase

Reaction equation

$$2\,\mathrm{ADP} \rightleftharpoons \mathrm{ATP} + \mathrm{AMP} \tag{29}$$

Reactant

Table 49: Properties of each reactant.

Id	Name	SBO
ADP		

Products

Table 50: Properties of each product.

Id	Name	SBO
ATP		
AMP		

Kinetic Law

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

$$v_{15} = \mathrm{vol}\,(\mathrm{cyto}) \cdot (\mathrm{k1\_15} \cdot [\mathrm{ADP}] \cdot [\mathrm{ADP}] - \mathrm{k2\_15} \cdot [\mathrm{ATP}] \cdot [\mathrm{AMP}]) \tag{30}$$

Table 51: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1_15			45.0	$\mathrm{mmol}^{-1} \cdot (60\ \mathrm{s})^{-1} \cdot \mathrm{l}$	☑

Id	Name	SBO	Value	Unit	Constant
k2_15			100.0	$\mathrm{mmol}^{-1} \cdot (60\ \mathrm{s})^{-1} \cdot \mathrm{l}$	☑

6.16 Reaction G3PDH

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

Name glycerol-3-phosphate_dehydrogenase

Reaction equation

$$\mathrm{DHAP} + \mathrm{NADH} \rightleftharpoons \mathrm{NAD} + \mathrm{Glycerol} \tag{31}$$

Reactants

Table 52: Properties of each reactant.

Id	Name	SBO
DHAP		
NADH		

Products

Table 53: Properties of each product.

Id	Name	SBO
NAD		
Glycerol		

Kinetic Law

Derived unit contains undeclared units

$$v_{16} = \frac{\mathrm{vol}\,(\mathrm{cyto}) \cdot \mathrm{Vmax\_16} \cdot \mathrm{WGD\_E} \cdot \left(\frac{[\mathrm{DHAP}]}{\mathrm{Kdhap\_16}} \cdot \frac{[\mathrm{NADH}]}{\mathrm{Knadh\_16}} - \frac{[\mathrm{Glycerol}]}{\mathrm{Kdhap\_16}} \cdot \frac{[\mathrm{NAD}]}{\mathrm{Knadh\_16}} \cdot \frac{1}{\mathrm{Keq\_16}} \right)}{\left(1 + \frac{[\mathrm{DHAP}]}{\mathrm{Kdhap\_16}} + \frac{[\mathrm{Glycerol}]}{\mathrm{Kglycerol\_16}} \right) \cdot \left(1 + \frac{[\mathrm{NADH}]}{\mathrm{Knadh\_16}} + \frac{[\mathrm{NAD}]}{\mathrm{Knad\_16}} \right)} \tag{32}$$

Table 54: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax_16			47.110	mmol · $(60\,\mathrm{s})^{-1}$ · l^{-1}	☑
Kdhap_16			0.400	$\mathrm{l}^{-1}\cdot$mmol	☑
Knadh_16			0.023	$\mathrm{l}^{-1}\cdot$mmol	☑
Keq_16			4300.000	dimensionless	☑
Kglycerol_16			1.000	$\mathrm{l}^{-1}\cdot$mmol	☑
Knad_16			0.930	$\mathrm{l}^{-1}\cdot$mmol	☑

6.17 Reaction glycogen_branch

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

Name glycogenbranch

Reaction equation

$$\mathrm{ATP} + \mathrm{G6P} \longrightarrow \mathrm{ADP} + \mathrm{Glycogen} \tag{33}$$

Reactants

Table 55: Properties of each reactant.

Id	Name	SBO
ATP		
G6P		

Products

Table 56: Properties of each product.

Id	Name	SBO
ADP		
Glycogen		

Kinetic Law

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

$$v_{17} = \mathrm{vol}\,(\mathrm{cyto}) \cdot \mathrm{KGLYCOGEN\_17} \tag{34}$$

Table 57: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
KGLYCOGEN_17			6.0	$\text{mmol} \cdot (60\,\text{s})^{-1} \cdot \text{l}^{-1}$	☑

6.18 Reaction trehalose_synth

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

Name trehalose_synthesis

Reaction equation

$$\text{ATP} + 2\,\text{G6P} \longrightarrow \text{ADP} + \text{Trehalose} \tag{35}$$

Reactants

Table 58: Properties of each reactant.

Id	Name	SBO
ATP		
G6P		

Products

Table 59: Properties of each product.

Id	Name	SBO
ADP		
Trehalose		

Kinetic Law

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

$$v_{18} = \text{vol}\,(\text{cyto}) \cdot \text{Ktrehalose\_18} \tag{36}$$

Table 60: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Ktrehalose_18			2.4	$\text{mmol} \cdot (60\,\text{s})^{-1} \cdot \text{l}^{-1}$	☑

6.19 Reaction succinate_syn

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

Name succinate_synthesis

Reaction equation

$$3\,\text{NAD} + 2\,\text{AcAld} \longrightarrow 3\,\text{NADH} + \text{Succinate} \tag{37}$$

Reactants

Table 61: Properties of each reactant.

Id	Name	SBO
NAD		
AcAld		

Products

Table 62: Properties of each product.

Id	Name	SBO
NADH		
Succinate		

Kinetic Law

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

$$v_{19} = \text{vol}\,(\text{cyto}) \cdot \text{k\_19} \cdot [\text{AcAld}] \tag{38}$$

Table 63: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k_19			21.4	$(60\ \mathrm{s})^{-1}$	☑

6.20 Reaction PYR_shut

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

Name pyruvate_shuttling

Reaction equation

$$\mathrm{PYR} \rightleftharpoons \mathrm{PYRmito} \tag{39}$$

Reactant

Table 64: Properties of each reactant.

Id	Name	SBO
PYR		

Product

Table 65: Properties of each product.

Id	Name	SBO
PYRmito		

Kinetic Law

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

$$v_{20} = \mathrm{t\_m} \cdot (\mathrm{k1} \cdot [\mathrm{PYR}] - \mathrm{k2} \cdot [\mathrm{PYRmito}]) \tag{40}$$

Table 66: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1			1.0	$1 \cdot (60\ \mathrm{s})^{-1}$	☑
k2			1.0	$1 \cdot (60\ \mathrm{s})^{-1}$	☑

6.21 Reaction PDH

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

Name pyruvate dehydrogenase

Reaction equation

$$\text{PYRmito} \xrightarrow{\text{NAD, NADH}} \text{AcCoA} + \text{CO2mito} \tag{41}$$

Reactant

Table 67: Properties of each reactant.

Id	Name	SBO
PYRmito		

Modifiers

Table 68: Properties of each modifier.

Id	Name	SBO
NAD		
NADH		

Products

Table 69: Properties of each product.

Id	Name	SBO
AcCoA		
CO2mito		

Kinetic Law

Derived unit contains undeclared units

$$v_{21} = \frac{\text{vol}(\text{mito}) \cdot \text{WGD\_E} \cdot \text{Vmax\_PDH} \cdot [\text{PYRmito}] \cdot \left(\text{NADX\_tot} - \frac{\text{NADX\_tot}}{1+\frac{[\text{NAD}]}{[\text{NADH}]}}\right)}{\frac{\text{NADX\_tot} \cdot \text{Ki\_PYR} \cdot \text{K\_NAD}}{\text{Ki\_NADH}} + \text{K\_PYR} \cdot \left(\text{NADX\_tot} - \frac{\text{NADX\_tot}}{1+\frac{[\text{NAD}]}{[\text{NADH}]}}\right) + \text{K\_NAD} \cdot [\text{PYRmito}] + \frac{\text{NADX\_tot} \cdot \text{K\_NAD} \cdot [\text{PYRmito}]}{\text{Ki\_NADH}} + \left(\text{NADX} \right.} \tag{42}$$

Table 70: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax_PDH			379.20	mmol · $(60\ \mathrm{s})^{-1}$ · l^{-1}	☑
NADX_tot	tot_NAD_in_mito		8.01	$\mathrm{l}^{-1} \cdot \mathrm{mmol}$	☑
K_PYR			70.00	$\mathrm{l}^{-1} \cdot \mathrm{mmol}$	☑
K_NAD			160.00	$\mathrm{l}^{-1} \cdot \mathrm{mmol}$	☑
Ki_NADH			50.00	$\mathrm{l}^{-1} \cdot \mathrm{mmol}$	☑
Ki_PYR			20.00	$\mathrm{l}^{-1} \cdot \mathrm{mmol}$	☑

7 Derived Rate Equations

When interpreted as an ordinary differential equation framework, this model implies the following set of equations for the rates of change of each species.

7.1 Species GLCi

Initial concentration $0.097652231064563\ \mathrm{mmol} \cdot \mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in HXK and as a product in HXT).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{GLCi} = v_1 - v_2 \tag{43}$$

7.2 Species ATP

Initial concentration $2.52512746499271\ \mathrm{mmol} \cdot \mathrm{l}^{-1}$

This species takes part in eight reactions (as a reactant in HXK, PFK, ATPase, glycogen_branch, trehalose_synth and as a product in PGK, PYK, AK).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ATP} = v_8 + v_{11} + v_{15} - v_2 - v_4 - v_{14} - v_{17} - v_{18} \tag{44}$$

7.3 Species G6P

Initial concentration $2.67504014044787\ \mathrm{mmol} \cdot \mathrm{l}^{-1}$

This species takes part in four reactions (as a reactant in PGI, glycogen_branch, trehalose_synth and as a product in HXK).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{G6P} = v_2 - v_3 - v_{17} - 2v_{18} \tag{45}$$

7.4 Species ADP

Initial concentration $1.28198768168719\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in eight reactions (as a reactant in PGK, PYK, AK and as a product in HXK, PFK, ATPase, glycogen_branch, trehalose_synth).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ADP} = v_2 + v_4 + v_{14} + v_{17} + v_{18} - v_8 - v_{11} - 2v_{15} \tag{46}$$

7.5 Species F6P

Initial concentration $0.624976405532373\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in PFK and as a product in PGI).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{F6P} = v_3 - v_4 \tag{47}$$

7.6 Species F16bP

Initial concentration $6.22132076069411\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in FBA and as a product in PFK).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{F16bP} = v_4 - v_5 \tag{48}$$

7.7 Species F26bP

Name Fru2,6-P2

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{F26bP} = 0 \tag{49}$$

7.8 Species AMP

Initial concentration $0.292884853320091\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a product in AK and as a modifier in PFK).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{AMP} = v_{15} \tag{50}$$

7.9 Species DHAP

Initial concentration $1.00415254899644\ \text{mmol}\cdot\text{l}^{-1}$

This species takes part in three reactions (as a reactant in TPI, G3PDH and as a product in FBA).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{DHAP} = v_5 - v_6 - v_{16} \tag{51}$$

7.10 Species GAP

Initial concentration $0.0451809175780963\ \text{mmol}\cdot\text{l}^{-1}$

This species takes part in three reactions (as a reactant in TDH and as a product in FBA, TPI).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{GAP} = v_5 + v_6 - v_7 \tag{52}$$

7.11 Species NAD

Initial concentration $1.50329030201531\ \text{mmol}\cdot\text{l}^{-1}$

This species takes part in five reactions (as a reactant in TDH, ADH, succinate_syn and as a product in G3PDH and as a modifier in PDH).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{NAD} = v_{16} - v_7 - v_{13} - 3v_{19} \tag{53}$$

7.12 Species BPG

Initial concentration $7.36873499865602 \cdot 10^{-4}\ \text{mmol}\cdot\text{l}^{-1}$

This species takes part in two reactions (as a reactant in PGK and as a product in TDH).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{BPG} = v_7 - v_8 \tag{54}$$

7.13 Species NADH

Initial concentration $0.0867096979846952\ \text{mmol}\cdot\text{l}^{-1}$

This species takes part in five reactions (as a reactant in G3PDH and as a product in TDH, ADH, succinate_syn and as a modifier in PDH).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{NADH} = v_7 + v_{13} + 3v_{19} - v_{16} \tag{55}$$

7.14 Species P3G

Initial concentration $0.885688538360659\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in PGM and as a product in PGK).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{P3G} = v_8 - v_9 \tag{56}$$

7.15 Species P2G

Initial concentration $0.127695817386632\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in ENO and as a product in PGM).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{P2G} = v_9 - v_{10} \tag{57}$$

7.16 Species PEP

Initial concentration $0.0632352144936527\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in PYK and as a product in ENO).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{PEP} = v_{10} - v_{11} \tag{58}$$

7.17 Species PYR

Initial concentration $1.81531251192736\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in three reactions (as a reactant in PDC, PYR_shut and as a product in PYK).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{PYR} = v_{11} - v_{12} - v_{20} \tag{59}$$

7.18 Species PYRmito

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

This species takes part in two reactions (as a reactant in PDH and as a product in PYR_shut).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{PYRmito} = v_{20} - v_{21} \tag{60}$$

7.19 Species AcAld

Initial concentration $0.178140579850657\ \text{mmol} \cdot \text{l}^{-1}$

This species takes part in three reactions (as a reactant in succinate_syn and as a product in PDC, ADH).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{AcAld} = v_{12} + v_{13} - 2v_{19} \tag{61}$$

7.20 Species GLCo

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

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:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{GLCo} = 0 \tag{62}$$

7.21 Species CO2

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{CO2} = 0 \tag{63}$$

7.22 Species EtOH

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

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

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

7.23 Species Glycerol

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

This species takes part in one reaction (as a product in G3PDH), which does not influence its rate of change because this species is on the boundary of the reaction system:

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

7.24 Species Glycogen

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

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

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

7.25 Species Trehalose

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

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

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

7.26 Species Succinate

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Succinate} = 0 \tag{68}$$

7.27 Species AcCoA

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{AcCoA} = 0 \tag{69}$$

7.28 Species CO2mito

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{CO2mito} = 0 \tag{70}$$

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