SBML Model Report

Model name: "Hynne2001_Glycolysis"

May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 1 format. This model was created by the following two authors: Jacky L Snoep[1] and Harish Dharuri[2] at July twelveth 2006 at 7:49 a. m. and last time modified at June third 2013 at 2:20 p. m. Table 1 shows an overview of the quantities of all components of this model.

Table 1: Number of components in this model, which are described in the following sections.

Element	Quantity	Element	Quantity
compartment types	0	compartments	2
species types	0	species	25
events	0	constraints	0
reactions	24	function definitions	0
global parameters	0	unit definitions	7
rules	0	initial assignments	0

Model Notes

The model reproduces Fig 6 of the paper. The stoichiometry and rate of reactions involving uptake of metabolites from extracellular medium have been changed corresponding to Yvol (ratio of extracellular volume to cytosolic volume) mentioned in the publication. The extracellular and cytosolic compartments have been set to 1. Concentration of extracellular glucose, GlcX, is set to 6.7 according to the equation for cellular glucose uptake rate in Table 7 of the paper. The model was successfully tested on MathSBML and Jarnac

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SBML level 2 code generated for the JWS Online project by Jacky Snoep using PySCeS
Run this model online at http://jjj.biochem.sun.ac.za
To cite JWS Online please refer to: Olivier, B.G. and Snoep, J.L. (2004) Web-based modelling using JWS Online , Bioinformatics, 20:2143-2144

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2 Unit Definitions

This is an overview of ten 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 `mM_per_minute`

Name mM per minute

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

2.4 Unit min_inverse

Name minute inverse

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

2.5 Unit mM_inverse_min_inverse

Name mM inverse min inverse

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

2.6 Unit mM_squared

Name mM squared

Definition $\mathrm{mmol}^{2} \cdot 1^{-2}$

2.7 Unit mM

Name milliMolar

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

2.8 Unit volume

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

Definition l

2.9 Unit area

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

Definition m^{2}

2.10 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`			3	1	litre	☑	
`cytosol`			3	1	litre	☑	`extracellular`

3.1 Compartment `extracellular`

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

3.2 Compartment `cytosol`

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

4 Species

This model contains 25 species. The boundary condition of three of these species is set to `true` so that these species' amount cannot be changed by any reaction. Section 6 provides further details and the derived rates of change of each species.

Table 3: Properties of each species.

Id	Name	Compartment	Derived Unit	Constant	Boundary Condition
GlcX	Extracellular glucose	extracellular	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Glc	Cytosolic glucose	cytosol	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
ATP	ATP	cytosol	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
G6P	Glucose-6-Phosphate	cytosol	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
ADP	ADP	cytosol	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
F6P	Fructose-6-Phosphate	cytosol	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
FBP	Fructose 1,6-bisphosphate	cytosol	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
GAP	Glyceraldehyde 3-phosphate	cytosol	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
DHAP	Dihydroxyacetone phosphate	cytosol	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
NAD	NAD	cytosol	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
BPG	1,3-Bisphosphoglycerate	cytosol	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
NADH	NADH	cytosol	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
PEP	Phosphoenolpyruvate	cytosol	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Pyr	Pyruvate	cytosol	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
ACA	Acetaldehyde	cytosol	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
EtOH		cytosol	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
EtOHX	Extracellular ethanol	extracellular	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Glyc	Glycerol	cytosol	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
GlycX	Extracellular glycerol	extracellular	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
ACAX	Extracellular acetaldehyde	extracellular	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
CNX	Extracellular cyanide	extracellular	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟

Id	Name	Compartment	Derived Unit	Constant	Boundary Condition
`AMP`	AMP	`cytosol`	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☐
`P`		`extracellular`	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☑
`CNX0`	Mixed flow cyanide	`extracellular`	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☑
`GlcX0`	Mixed flow glucose	`extracellular`	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☑

5 Reactions

This model contains 24 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 4: Overview of all reactions

№	Id	Name	Reaction Equation	SBO
1	vinGlc	Glucose Mixed flow to extracellular medium	$\mathrm{GlcX0} \rightleftharpoons \mathrm{GlcX}$	
2	vGlcTrans	Glucose uptake	$\mathrm{GlcX} \overset{\mathrm{G6P}}{\rightleftharpoons} 59\,\mathrm{Glc}$	
3	vHK	Hexokinase	$\mathrm{ATP} + \mathrm{Glc} \rightleftharpoons \mathrm{G6P} + \mathrm{ADP}$	
4	vPGI	Phosphoglucoisomerase	$\mathrm{G6P} \rightleftharpoons \mathrm{F6P}$	
5	vPFK	Phosphofructokinase	$\mathrm{F6P} + \mathrm{ATP} \overset{\mathrm{AMP}}{\rightleftharpoons} \mathrm{FBP} + \mathrm{ADP}$	
6	vALD	Aldolase	$\mathrm{FBP} \rightleftharpoons \mathrm{GAP} + \mathrm{DHAP}$	
7	vTIM	Triosephosphate isomerase	$\mathrm{DHAP} \rightleftharpoons \mathrm{GAP}$	
8	vGAPDH	Glyceraldehyde 3-phosphate dehydrogenase	$\mathrm{GAP} + \mathrm{NAD} \rightleftharpoons \mathrm{NADH} + \mathrm{BPG}$	
9	vlpPEP	Phosphoenolpyruvate synthesis	$\mathrm{BPG} + \mathrm{ADP} \rightleftharpoons \mathrm{PEP} + \mathrm{ATP}$	
10	vPK	Pyruvate kinase	$\mathrm{ADP} + \mathrm{PEP} \rightleftharpoons \mathrm{Pyr} + \mathrm{ATP}$	
11	vPDC	Pyruvate decarboxylase	$\mathrm{Pyr} \rightleftharpoons \mathrm{ACA}$	
12	vADH	Alcohol dehydrogenase	$\mathrm{NADH} + \mathrm{ACA} \rightleftharpoons \mathrm{NAD} + \mathrm{EtOH}$	
13	vdifEtOH	Ethanol out	$59\,\mathrm{EtOH} \rightleftharpoons \mathrm{EtOHX}$	
14	voutEtOH	Ethanol flow	$\mathrm{EtOHX} \rightleftharpoons \mathrm{P}$	
15	vlpGlyc	Glycerol synthesis	$\mathrm{DHAP} + \mathrm{NADH} \rightleftharpoons \mathrm{Glyc} + \mathrm{NAD}$	
16	vdifGlyc	Glycerol out	$59\,\mathrm{Glyc} \rightleftharpoons \mathrm{GlycX}$	
17	voutGlyc	Glycerol flow	$\mathrm{GlycX} \rightleftharpoons \mathrm{P}$	
18	vdifACA	Acetaldehyde out	$59\,\mathrm{ACA} \rightleftharpoons \mathrm{ACAX}$	
19	voutACA	Acetaldehyde flow	$\mathrm{ACAX} \rightleftharpoons \mathrm{P}$	
20	vlacto	Cyanide-Acetaldehyde flow	$\mathrm{CNX} + \mathrm{ACAX} \rightleftharpoons \mathrm{P}$	
21	vinCN	Cyanide flow	$\mathrm{CNX0} \rightleftharpoons \mathrm{CNX}$	
22	vstorage	Storage	$\mathrm{ATP} + \mathrm{G6P} \rightleftharpoons \mathrm{ADP}$	

№	Id	Name	Reaction Equation	SBO
23	vconsum	ATP consumption	$\mathrm{ATP} \rightleftharpoons \mathrm{ADP}$	
24	vAK	Adenylate kinase	$\mathrm{ATP} + \mathrm{AMP} \rightleftharpoons 2\,\mathrm{ADP}$	

5.1 Reaction vinGlc

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

Name Glucose Mixed flow to extracellular medium

Reaction equation

$$\mathrm{GlcX0} \rightleftharpoons \mathrm{GlcX} \tag{1}$$

Reactant

Table 5: Properties of each reactant.

Id	Name	SBO
GlcX0	Mixed flow glucose	

Product

Table 6: Properties of each product.

Id	Name	SBO
GlcX	Extracellular glucose	

Kinetic Law

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

$$v_1 = \mathrm{vol}\,(\mathrm{extracellular}) \cdot \mathrm{k0} \cdot ([\mathrm{GlcX0}] - [\mathrm{GlcX}]) \tag{2}$$

Table 7: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k0			0.048	$(60\ \mathrm{s})^{-1}$	☑

5.2 Reaction vGlcTrans

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

Name Glucose uptake

Reaction equation

$$\mathrm{GlcX} \underset{\longleftarrow}{\overset{\mathrm{G6P}}{\rightleftharpoons}} 59\,\mathrm{Glc} \tag{3}$$

Reactant

Table 8: Properties of each reactant.

Id	Name	SBO
`GlcX`	Extracellular glucose	

Modifier

Table 9: Properties of each modifier.

Id	Name	SBO
`G6P`	Glucose-6-Phosphate	

Product

Table 10: Properties of each product.

Id	Name	SBO
`Glc`	Cytosolic glucose	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \frac{\mathrm{vol}\,(\mathrm{extracellular}) \cdot \mathrm{V2f}}{\mathrm{Yvol}} \cdot \frac{\frac{[\mathrm{GlcX}]}{\mathrm{K2Glc}}}{1 + \frac{[\mathrm{GlcX}]}{\mathrm{K2Glc}} + \frac{\mathrm{P2} \cdot \frac{[\mathrm{GlcX}]}{\mathrm{K2Glc}} + 1}{\mathrm{P2} \cdot \frac{[\mathrm{Glc}]}{\mathrm{K2Glc}} + 1} \cdot \left(1 + \frac{[\mathrm{Glc}]}{\mathrm{K2Glc}} + \frac{[\mathrm{G6P}]}{\mathrm{K2IG6P}} + \frac{[\mathrm{Glc}] \cdot [\mathrm{G6P}]}{\mathrm{K2Glc} \cdot \mathrm{K2IIG6P}}\right)}$$
$$- \frac{\mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{V2r}}{\mathrm{Yvol}} \cdot \frac{\frac{[\mathrm{Glc}]}{\mathrm{K2Glc}}}{1 + \frac{[\mathrm{Glc}]}{\mathrm{K2Glc}} + \frac{\mathrm{P2} \cdot \frac{[\mathrm{Glc}]}{\mathrm{K2Glc}} + 1}{\mathrm{P2} \cdot \frac{[\mathrm{GlcX}]}{\mathrm{K2Glc}} + 1} \cdot \left(1 + \frac{[\mathrm{GlcX}]}{\mathrm{K2Glc}}\right) + \frac{[\mathrm{G6P}]}{\mathrm{K2IG6P}} + \frac{[\mathrm{Glc}] \cdot [\mathrm{G6P}]}{\mathrm{K2Glc} \cdot \mathrm{K2IIG6P}}} \tag{4}$$

Table 11: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V2f			1014.96	mmol · l^{-1} · $(60\ s)^{-1}$	☑
Yvol			59.00	dimensionless	☑
K2Glc			1.70	mmol · l^{-1}	☑
P2			1.00	dimensionless	☑
K2IG6P			1.20	mmol · l^{-1}	☑
K2IIG6P			7.20	mmol · l^{-1}	☑
V2r			1014.96	mmol · l^{-1} · $(60\ s)^{-1}$	☑

5.3 Reaction vHK

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

Name Hexokinase

Reaction equation

$$\mathrm{ATP} + \mathrm{Glc} \rightleftharpoons \mathrm{G6P} + \mathrm{ADP} \tag{5}$$

Reactants

Table 12: Properties of each reactant.

Id	Name	SBO
ATP	ATP	
Glc	Cytosolic glucose	

Products

Table 13: Properties of each product.

Id	Name	SBO
G6P	Glucose-6-Phosphate	
ADP	ADP	

Kinetic Law

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

$$v_3 = \frac{\text{vol}\,(\text{cytosol}) \cdot \text{V3m} \cdot [\text{ATP}] \cdot [\text{Glc}]}{\text{K3DGlc} \cdot \text{K3ATP} + \text{K3Glc} \cdot [\text{ATP}] + \text{K3ATP} \cdot [\text{Glc}] + [\text{Glc}] \cdot [\text{ATP}]} \tag{6}$$

Table 14: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V3m			51.755	$\text{mmol} \cdot \text{l}^{-1} \cdot (60\ \text{s})^{-1}$	☑
K3DGlc			0.370	$\text{mmol} \cdot \text{l}^{-1}$	☑
K3ATP			0.100	$\text{mmol} \cdot \text{l}^{-1}$	☑
K3Glc			0.000	$\text{mmol} \cdot \text{l}^{-1}$	☑

5.4 Reaction vPGI

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

Name Phosphoglucoisomerase

Reaction equation

$$\text{G6P} \rightleftharpoons \text{F6P} \tag{7}$$

Reactant

Table 15: Properties of each reactant.

Id	Name	SBO
G6P	Glucose-6-Phosphate	

Product

Table 16: Properties of each product.

Id	Name	SBO
F6P	Fructose-6-Phosphate	

Kinetic Law

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

$$v_4 = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \left(\frac{\mathrm{V4f} \cdot [\mathrm{G6P}]}{\mathrm{K4G6P} + [\mathrm{G6P}] + \frac{\mathrm{K4G6P}}{\mathrm{K4F6P}} \cdot [\mathrm{F6P}]} - \frac{\mathrm{V4r} \cdot \frac{[\mathrm{F6P}]}{\mathrm{K4eq}}}{\mathrm{K4G6P} + [\mathrm{G6P}] + \frac{\mathrm{K4G6P}}{\mathrm{K4F6P}} \cdot [\mathrm{F6P}]} \right) \tag{8}$$

Table 17: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V4f			496.042	$\mathrm{mmol} \cdot \mathrm{l}^{-1} \cdot (60\ \mathrm{s})^{-1}$	☑
K4G6P			0.800	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
K4F6P			0.150	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
V4r			496.042	$\mathrm{mmol} \cdot \mathrm{l}^{-1} \cdot (60\ \mathrm{s})^{-1}$	☑
K4eq			0.130	dimensionless	☑

5.5 Reaction vPFK

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

Name Phosphofructokinase

Reaction equation

$$\mathrm{F6P} + \mathrm{ATP} \overset{\mathrm{AMP}}{\rightleftharpoons} \mathrm{FBP} + \mathrm{ADP} \tag{9}$$

Reactants

Table 18: Properties of each reactant.

Id	Name	SBO
F6P	Fructose-6-Phosphate	
ATP	ATP	

Modifier

Table 19: Properties of each modifier.

Id	Name	SBO
AMP	AMP	

Products

Table 20: Properties of each product.

Id	Name	SBO
FBP	Fructose 1,6-bisphosphate	
ADP	ADP	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \frac{\mathrm{V5m} \cdot [\mathrm{F6P}]^2}{\mathrm{K5} \cdot \left(1 + \mathrm{kappa5} \cdot \frac{[\mathrm{ATP}]}{[\mathrm{AMP}]} \cdot \frac{[\mathrm{ATP}]}{[\mathrm{AMP}]}\right) + [\mathrm{F6P}]^2} \tag{10}$$

Table 21: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V5m			45.433	$\mathrm{mmol} \cdot \mathrm{l}^{-1} \cdot (60\ \mathrm{s})^{-1}$	☑
K5			0.021	$\mathrm{mmol}^2 \cdot \mathrm{l}^{-2}$	☑
kappa5			0.150	dimensionless	☑

5.6 Reaction vALD

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

Name Aldolase

Reaction equation

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

Reactant

Table 22: Properties of each reactant.

Id	Name	SBO
FBP	Fructose 1,6-bisphosphate	

Products

Table 23: Properties of each product.

Id	Name	SBO
GAP	Glyceraldehyde 3-phosphate	
DHAP	Dihydroxyacetone phosphate	

Kinetic Law

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

$$v_6 = \mathrm{vol}(\mathrm{cytosol}) \cdot \left(\frac{\mathrm{V6f} \cdot [\mathrm{FBP}]}{\mathrm{K6FBP} + [\mathrm{FBP}] + \frac{[\mathrm{GAP}] \cdot \mathrm{K6DHAP} \cdot \mathrm{V6f}}{\mathrm{K6eq} \cdot \mathrm{V6f} \cdot \mathrm{ratio6}} + \frac{[\mathrm{DHAP}] \cdot \mathrm{K6GAP} \cdot \mathrm{V6f}}{\mathrm{K6eq} \cdot \mathrm{V6f} \cdot \mathrm{ratio6}} + \frac{[\mathrm{FBP}] \cdot [\mathrm{GAP}]}{\mathrm{K6IGAP}} + \frac{[\mathrm{GAP}] \cdot [\mathrm{DHAP}] \cdot \mathrm{V6f}}{\mathrm{K6eq} \cdot \mathrm{V6f} \cdot \mathrm{ratio6}}} - \frac{\frac{\mathrm{V6f} \cdot [\mathrm{GAP}] \cdot [\mathrm{DHAP}]}{\mathrm{K6eq}}}{\mathrm{K6FBP} + [\mathrm{FBP}] + \frac{[\mathrm{GAP}] \cdot \mathrm{K6DHAP} \cdot \mathrm{V6f}}{\mathrm{K6eq} \cdot \mathrm{V6f} \cdot \mathrm{ratio6}} + \frac{[\mathrm{DHAP}] \cdot \mathrm{K6GAP} \cdot \mathrm{V6f}}{\mathrm{K6eq} \cdot \mathrm{V6f} \cdot \mathrm{ratio6}} + \frac{[\mathrm{FBP}] \cdot [\mathrm{GAP}]}{\mathrm{K6IGAP}} + \frac{[\mathrm{GAP}] \cdot [\mathrm{DHAP}] \cdot \mathrm{V6f}}{\mathrm{K6eq} \cdot \mathrm{V6f} \cdot \mathrm{ratio6}}} \right) \tag{12}$$

Table 24: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V6f			2207.820	$\mathrm{mmol} \cdot \mathrm{l}^{-1} \cdot (60\ \mathrm{s})^{-1}$	☑
K6FBP			0.300	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
K6DHAP			2.000	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
K6eq			0.081	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
ratio6			5.000	dimensionless	☑
K6GAP			4.000	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
K6IGAP			10.000	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑

5.7 Reaction vTIM

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

Name Triosephosphate isomerase

Reaction equation

$$\mathrm{DHAP} \rightleftharpoons \mathrm{GAP} \tag{13}$$

Reactant

Table 25: Properties of each reactant.

Id	Name	SBO
DHAP	Dihydroxyacetone phosphate	

Product

Table 26: Properties of each product.

Id	Name	SBO
GAP	Glyceraldehyde 3-phosphate	

Kinetic Law

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

$$v_7 = \mathrm{vol}\,(\mathrm{cytosol})\cdot\left(\frac{\mathrm{V7f}\cdot[\mathrm{DHAP}]}{\mathrm{K7DHAP}+[\mathrm{DHAP}]+\frac{\mathrm{K7DHAP}}{\mathrm{K7GAP}}\cdot[\mathrm{GAP}]} - \frac{\mathrm{V7r}\cdot\frac{[\mathrm{GAP}]}{\mathrm{K7eq}}}{\mathrm{K7DHAP}+[\mathrm{DHAP}]+\frac{\mathrm{K7DHAP}}{\mathrm{K7GAP}}\cdot[\mathrm{GAP}]}\right) \tag{14}$$

Table 27: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V7f			116.365	$\mathrm{mmol}\cdot\mathrm{l}^{-1}\cdot(60\,\mathrm{s})^{-1}$	☑
K7DHAP			1.230	$\mathrm{mmol}\cdot\mathrm{l}^{-1}$	☑
K7GAP			1.270	$\mathrm{mmol}\cdot\mathrm{l}^{-1}$	☑
V7r			116.365	$\mathrm{mmol}\cdot\mathrm{l}^{-1}\cdot(60\,\mathrm{s})^{-1}$	☑
K7eq			0.055	dimensionless	☑

5.8 Reaction vGAPDH

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

Name Glyceraldehyde 3-phosphate dehydrogenase

Reaction equation

$$\mathrm{GAP} + \mathrm{NAD} \rightleftharpoons \mathrm{NADH} + \mathrm{BPG} \tag{15}$$

Reactants

Table 28: Properties of each reactant.

Id	Name	SBO
GAP	Glyceraldehyde 3-phosphate	
NAD	NAD	

Products

Table 29: Properties of each product.

Id	Name	SBO
NADH	NADH	
BPG	1,3-Bisphosphoglycerate	

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \left(\frac{\frac{\frac{\mathrm{V8f} \cdot [\mathrm{GAP}] \cdot [\mathrm{NAD}]}{\mathrm{K8GAP}}}{\mathrm{K8NAD}}}{\left(1 + \frac{[\mathrm{GAP}]}{\mathrm{K8GAP}} + \frac{[\mathrm{BPG}]}{\mathrm{K8BPG}}\right) \cdot \left(1 + \frac{[\mathrm{NAD}]}{\mathrm{K8NAD}} + \frac{[\mathrm{NADH}]}{\mathrm{K8NADH}}\right)} - \frac{\frac{\frac{\frac{\mathrm{V8r} \cdot [\mathrm{BPG}] \cdot [\mathrm{NADH}]}{\mathrm{K8eq}}}{\mathrm{K8GAP}}}{\mathrm{K8NAD}}}{\left(1 + \frac{[\mathrm{GAP}]}{\mathrm{K8GAP}} + \frac{[\mathrm{BPG}]}{\mathrm{K8BPG}}\right) \cdot \left(1 + \frac{[\mathrm{NAD}]}{\mathrm{K8NAD}} + \frac{[\mathrm{NADH}]}{\mathrm{K8NADH}}\right)} \right) \tag{16}$$

Table 30: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V8f			833.858	$\mathrm{mmol} \cdot \mathrm{l}^{-1} \cdot (60\ \mathrm{s})^{-1}$	☑
K8GAP			0.600	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑

Id	Name	SBO	Value	Unit	Constant
K8NAD			0.100	$\mathrm{mmol}\cdot\mathrm{l}^{-1}$	☑
K8BPG			0.010	$\mathrm{mmol}\cdot\mathrm{l}^{-1}$	☑
K8NADH			0.060	$\mathrm{mmol}\cdot\mathrm{l}^{-1}$	☑
V8r			833.858	$\mathrm{mmol}\cdot\mathrm{l}^{-1}\cdot(60\,\mathrm{s})^{-1}$	☑
K8eq			0.006	dimensionless	☑

5.9 Reaction vlpPEP

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

Name Phosphoenolpyruvate synthesis

Reaction equation

$$\mathrm{BPG} + \mathrm{ADP} \rightleftharpoons \mathrm{PEP} + \mathrm{ATP} \tag{17}$$

Reactants

Table 31: Properties of each reactant.

Id	Name	SBO
BPG	1,3-Bisphosphoglycerate	
ADP	ADP	

Products

Table 32: Properties of each product.

Id	Name	SBO
PEP	Phosphoenolpyruvate	
ATP	ATP	

Kinetic Law

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

$$v_9 = \mathrm{vol}\,(\mathrm{cytosol}) \cdot (\mathrm{k9f} \cdot [\mathrm{BPG}] \cdot [\mathrm{ADP}] - \mathrm{k9r} \cdot [\mathrm{PEP}] \cdot [\mathrm{ATP}]) \tag{18}$$

Table 33: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k9f			443866.00	$\text{mmol}^{-1} \cdot \text{l} \cdot (60\ \text{s})^{-1}$	☑
k9r			1528.62	$\text{mmol}^{-1} \cdot \text{l} \cdot (60\ \text{s})^{-1}$	☑

5.10 Reaction vPK

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

Name Pyruvate kinase

Reaction equation

$$\text{ADP} + \text{PEP} \rightleftharpoons \text{Pyr} + \text{ATP} \tag{19}$$

Reactants

Table 34: Properties of each reactant.

Id	Name	SBO
ADP	ADP	
PEP	Phosphoenolpyruvate	

Products

Table 35: Properties of each product.

Id	Name	SBO
Pyr	Pyruvate	
ATP	ATP	

Kinetic Law

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

$$v_{10} = \text{vol}\,(\text{cytosol}) \cdot \frac{\text{V10m} \cdot [\text{ADP}] \cdot [\text{PEP}]}{(\text{K10PEP} + [\text{PEP}]) \cdot (\text{K10ADP} + [\text{ADP}])} \tag{20}$$

Table 36: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V10m			343.096	$\text{mmol} \cdot \text{l}^{-1} \cdot (60\ \text{s})^{-1}$	☑
K10PEP			0.200	$\text{mmol} \cdot \text{l}^{-1}$	☑
K10ADP			0.170	$\text{mmol} \cdot \text{l}^{-1}$	☑

5.11 Reaction vPDC

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

Name Pyruvate decarboxylase

Reaction equation

$$\text{Pyr} \rightleftharpoons \text{ACA} \tag{21}$$

Reactant

Table 37: Properties of each reactant.

Id	Name	SBO
Pyr	Pyruvate	

Product

Table 38: Properties of each product.

Id	Name	SBO
ACA	Acetaldehyde	

Kinetic Law

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

$$v_{11} = \text{vol}\,(\text{cytosol}) \cdot \frac{\text{V11m} \cdot [\text{Pyr}]}{\text{K11} + [\text{Pyr}]} \tag{22}$$

Table 39: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V11m			53.133	$\text{mmol} \cdot \text{l}^{-1} \cdot (60\ \text{s})^{-1}$	☑
K11			0.300	$\text{mmol} \cdot \text{l}^{-1}$	☑

5.12 Reaction vADH

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

Name Alcohol dehydrogenase

Reaction equation

$$\text{NADH} + \text{ACA} \rightleftharpoons \text{NAD} + \text{EtOH} \tag{23}$$

Reactants

Table 40: Properties of each reactant.

Id	Name	SBO
NADH	NADH	
ACA	Acetaldehyde	

Products

Table 41: Properties of each product.

Id	Name	SBO
NAD	NAD	
EtOH		

Kinetic Law

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

$$v_{12} = \text{vol}(\text{cytosol}) \cdot \frac{\text{V12m} \cdot [\text{ACA}] \cdot [\text{NADH}]}{(\text{K12NADH} + [\text{NADH}]) \cdot (\text{K12ACA} + [\text{ACA}])} \tag{24}$$

Table 42: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V12m			89.802	mmol · l^{-1} · $(60\ s)^{-1}$	☑
K12NADH			0.100	mmol · l^{-1}	☑
K12ACA			0.710	mmol · l^{-1}	☑

5.13 Reaction vdifEtOH

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

Name Ethanol out

Reaction equation

$$59\,\mathrm{EtOH} \rightleftharpoons \mathrm{EtOHX} \tag{25}$$

Reactant

Table 43: Properties of each reactant.

Id	Name	SBO
EtOH		

Product

Table 44: Properties of each product.

Id	Name	SBO
EtOHX	Extracellular ethanol	

Kinetic Law

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

$$v_{13} = \frac{\mathrm{k13}}{\mathrm{Yvol}} \cdot (\mathrm{vol}\,(\mathrm{cytosol}) \cdot [\mathrm{EtOH}] - \mathrm{vol}\,(\mathrm{extracellular}) \cdot [\mathrm{EtOHX}]) \tag{26}$$

Table 45: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k13			16.72	$(60\ \mathrm{s})^{-1}$	☑
Yvol			59.00	dimensionless	☑

5.14 Reaction voutEtOH

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

Name Ethanol flow

Reaction equation

$$\mathrm{EtOHX} \rightleftharpoons \mathrm{P} \tag{27}$$

Reactant

Table 46: Properties of each reactant.

Id	Name	SBO
EtOHX	Extracellular ethanol	

Product

Table 47: Properties of each product.

Id	Name	SBO
P		

Kinetic Law

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

$$v_{14} = \mathrm{vol}\,(\mathrm{extracellular}) \cdot \mathrm{k0} \cdot [\mathrm{EtOHX}] \tag{28}$$

Table 48: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k0			0.048	$(60\ \mathrm{s})^{-1}$	☑

5.15 Reaction `vlpGlyc`

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

Name Glycerol synthesis

Reaction equation

$$\mathrm{DHAP} + \mathrm{NADH} \rightleftharpoons \mathrm{Glyc} + \mathrm{NAD} \tag{29}$$

Reactants

Table 49: Properties of each reactant.

Id	Name	SBO
`DHAP`	Dihydroxyacetone phosphate	
`NADH`	NADH	

Products

Table 50: Properties of each product.

Id	Name	SBO
`Glyc`	Glycerol	
`NAD`	NAD	

Kinetic Law

Derived unit contains undeclared units

$$v_{15} = \mathrm{vol}(\mathrm{cytosol}) \cdot \frac{\mathrm{V15m} \cdot [\mathrm{DHAP}]}{\mathrm{K15DHAP} \cdot \left(1 + \frac{\mathrm{K15INADH}}{[\mathrm{NADH}]} \cdot \left(1 + \frac{[\mathrm{NAD}]}{\mathrm{K15INAD}}\right)\right) + [\mathrm{DHAP}] \cdot \left(1 + \frac{\mathrm{K15NADH}}{[\mathrm{NADH}]} \cdot \left(1 + \frac{[\mathrm{NAD}]}{\mathrm{K15INAD}}\right)\right)} \tag{30}$$

Table 51: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
`V15m`			81.480	$\mathrm{mmol} \cdot \mathrm{l}^{-1} \cdot (60\ \mathrm{s})^{-1}$	☑
`K15DHAP`			25.000	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
`K15INADH`			0.034	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑

Id	Name	SBO	Value	Unit	Constant
K15INAD			0.130	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
K15NADH			0.130	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑

5.16 Reaction vdifGlyc

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

Name Glycerol out

Reaction equation

$$59\,\mathrm{Glyc} \rightleftharpoons \mathrm{GlycX} \tag{31}$$

Reactant

Table 52: Properties of each reactant.

Id	Name	SBO
Glyc	Glycerol	

Product

Table 53: Properties of each product.

Id	Name	SBO
GlycX	Extracellular glycerol	

Kinetic Law

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

$$v_{16} = \frac{\mathrm{k16}}{\mathrm{Yvol}} \cdot (\mathrm{vol}\,(\mathrm{cytosol}) \cdot [\mathrm{Glyc}] - \mathrm{vol}\,(\mathrm{extracellular}) \cdot [\mathrm{GlycX}]) \tag{32}$$

Table 54: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k16			1.9	$(60\,\mathrm{s})^{-1}$	☑
Yvol			59.0	dimensionless	☑

5.17 Reaction voutGlyc

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

Name Glycerol flow

Reaction equation

$$\text{GlycX} \rightleftharpoons \text{P} \tag{33}$$

Reactant

Table 55: Properties of each reactant.

Id	Name	SBO
GlycX	Extracellular glycerol	

Product

Table 56: Properties of each product.

Id	Name	SBO
P		

Kinetic Law

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

$$v_{17} = \text{vol}\,(\text{extracellular}) \cdot \text{k0} \cdot [\text{GlycX}] \tag{34}$$

Table 57: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k0			0.048	$(60\ \text{s})^{-1}$	☑

5.18 Reaction vdifACA

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

Name Acetaldehyde out

Reaction equation

$$59\,\mathrm{ACA} \rightleftharpoons \mathrm{ACAX} \tag{35}$$

Reactant

Table 58: Properties of each reactant.

Id	Name	SBO
ACA	Acetaldehyde	

Product

Table 59: Properties of each product.

Id	Name	SBO
ACAX	Extracellular acetaldehyde	

Kinetic Law

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

$$v_{18} = \frac{\mathrm{k18}}{\mathrm{Yvol}} \cdot (\mathrm{vol}\,(\mathrm{cytosol}) \cdot [\mathrm{ACA}] - \mathrm{vol}\,(\mathrm{extracellular}) \cdot [\mathrm{ACAX}]) \tag{36}$$

Table 60: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k18			24.7	$(60\,\mathrm{s})^{-1}$	☑
Yvol			59.0	dimensionless	☑

5.19 Reaction voutACA

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

Name Acetaldehyde flow

Reaction equation

$$\mathrm{ACAX} \rightleftharpoons \mathrm{P} \tag{37}$$

Reactant

Table 61: Properties of each reactant.

Id	Name	SBO
ACAX	Extracellular acetaldehyde	

Product

Table 62: Properties of each product.

Id	Name	SBO
P		

Kinetic Law

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

$$v_{19} = \mathrm{vol}\,(\mathrm{extracellular}) \cdot \mathrm{k0} \cdot [\mathrm{ACAX}] \tag{38}$$

Table 63: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k0			0.048	$(60\ \mathrm{s})^{-1}$	☑

5.20 Reaction vlacto

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

Name Cyanide-Acetaldehyde flow

Reaction equation

$$\mathrm{CNX} + \mathrm{ACAX} \rightleftharpoons \mathrm{P} \tag{39}$$

Reactants

Table 64: Properties of each reactant.

Id	Name	SBO
CNX	Extracellular cyanide	

Id	Name	SBO
ACAX	Extracellular acetaldehyde	

Product

Table 65: Properties of each product.

Id	Name	SBO
P		

Kinetic Law

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

$$v_{20} = \mathrm{vol}\,(\mathrm{extracellular}) \cdot \mathrm{k20} \cdot [\mathrm{ACAX}] \cdot [\mathrm{CNX}] \tag{40}$$

Table 66: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k20			0.003	$\mathrm{mmol}^{-1} \cdot 1 \cdot (60\ \mathrm{s})^{-1}$	☑

5.21 Reaction vinCN

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

Name Cyanide flow

Reaction equation

$$\mathrm{CNX0} \rightleftharpoons \mathrm{CNX} \tag{41}$$

Reactant

Table 67: Properties of each reactant.

Id	Name	SBO
CNX0	Mixed flow cyanide	

Product

Table 68: Properties of each product.

Id	Name	SBO
CNX	Extracellular cyanide	

Kinetic Law

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

$$v_{21} = \mathrm{vol}\,(\mathrm{extracellular}) \cdot \mathrm{k0} \cdot ([\mathrm{CNX0}] - [\mathrm{CNX}]) \tag{42}$$

Table 69: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k0			0.048	$(60\ \mathrm{s})^{-1}$	☑

5.22 Reaction vstorage

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

Name Storage

Reaction equation

$$\mathrm{ATP} + \mathrm{G6P} \rightleftharpoons \mathrm{ADP} \tag{43}$$

Reactants

Table 70: Properties of each reactant.

Id	Name	SBO
ATP	ATP	
G6P	Glucose-6-Phosphate	

Product

Table 71: Properties of each product.

Id	Name	SBO
ADP	ADP	

Kinetic Law

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

$$v_{22} = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{k22} \cdot [\mathrm{ATP}] \cdot [\mathrm{G6P}] \tag{44}$$

Table 72: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k22			2.259	$\mathrm{mmol}^{-1} \cdot \mathrm{l} \cdot (60\ \mathrm{s})^{-1}$	☑

5.23 Reaction vconsum

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

Name ATP consumption

Reaction equation

$$\mathrm{ATP} \rightleftharpoons \mathrm{ADP} \tag{45}$$

Reactant

Table 73: Properties of each reactant.

Id	Name	SBO
ATP	ATP	

Product

Table 74: Properties of each product.

Id	Name	SBO
ADP	ADP	

Kinetic Law

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

$$v_{23} = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \mathrm{k23} \cdot [\mathrm{ATP}] \tag{46}$$

Table 75: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k23			3.208	$(60\ \mathrm{s})^{-1}$	☑

5.24 Reaction vAK

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

Name Adenylate kinase

Reaction equation

$$\mathrm{ATP} + \mathrm{AMP} \rightleftharpoons 2\,\mathrm{ADP} \tag{47}$$

Reactants

Table 76: Properties of each reactant.

Id	Name	SBO
ATP	ATP	
AMP	AMP	

Product

Table 77: Properties of each product.

Id	Name	SBO
ADP	ADP	

Kinetic Law

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

$$v_{24} = \mathrm{vol}\,(\mathrm{cytosol}) \cdot \left(\mathrm{k24f} \cdot [\mathrm{AMP}] \cdot [\mathrm{ATP}] - \mathrm{k24r} \cdot [\mathrm{ADP}]^2\right) \tag{48}$$

Table 78: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k24f			432.900	$\mathrm{mmol}^{-1} \cdot \mathrm{l} \cdot (60\ \mathrm{s})^{-1}$	☑

Id	Name	SBO	Value	Unit	Constant
k24r			133.333	$\text{mmol}^{-1} \cdot \text{l} \cdot (60\ \text{s})^{-1}$	☑

6 Derived Rate Equations

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

6.1 Species GlcX

Name Extracellular glucose

Initial concentration $6.7\ \text{mmol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a reactant in vGlcTrans and as a product in vinGlc).

$$\frac{\text{d}}{\text{d}t}\text{GlcX} = v_1 - v_2 \tag{49}$$

6.2 Species Glc

Name Cytosolic glucose

Initial concentration $0.573074\ \text{mmol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a reactant in vHK and as a product in vGlcTrans).

$$\frac{\text{d}}{\text{d}t}\text{Glc} = 59v_2 - v_3 \tag{50}$$

6.3 Species ATP

Name ATP

Initial concentration $2.1\ \text{mmol} \cdot \text{l}^{-1}$

This species takes part in seven reactions (as a reactant in vHK, vPFK, vstorage, vconsum, vAK and as a product in vlpPEP, vPK).

$$\frac{\text{d}}{\text{d}t}\text{ATP} = v_9 + v_{10} - v_3 - v_5 - v_{22} - v_{23} - v_{24} \tag{51}$$

6.4 Species G6P

Name Glucose-6-Phosphate

Initial concentration $4.2\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in four reactions (as a reactant in vPGI, vstorage and as a product in vHK and as a modifier in vGlcTrans).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{G6P} = v_3 - v_4 - v_{22} \tag{52}$$

6.5 Species ADP

Name ADP

Initial concentration $1.5\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in seven reactions (as a reactant in vlpPEP, vPK and as a product in vHK, vPFK, vstorage, vconsum, vAK).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ADP} = v_3 + v_5 + v_{22} + v_{23} + 2v_{24} - v_9 - v_{10} \tag{53}$$

6.6 Species F6P

Name Fructose-6-Phosphate

Initial concentration $0.49\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{F6P} = v_4 - v_5 \tag{54}$$

6.7 Species FBP

Name Fructose 1,6-bisphosphate

Initial concentration $4.64\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{FBP} = v_5 - v_6 \tag{55}$$

6.8 Species GAP

Name Glyceraldehyde 3-phosphate

Initial concentration $0.115\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{GAP} = v_6 + v_7 - v_8 \tag{56}$$

6.9 Species DHAP

Name Dihydroxyacetone phosphate

Initial concentration $2.95\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{DHAP} = v_6 - v_7 - v_{15} \tag{57}$$

6.10 Species NAD

Name NAD

Initial concentration $0.65\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{NAD} = v_{12} + v_{15} - v_8 \tag{58}$$

6.11 Species BPG

Name 1,3-Bisphosphoglycerate

Initial concentration $2.7\cdot 10^{-4}\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{BPG} = v_8 - v_9 \tag{59}$$

6.12 Species NADH

Name NADH

Initial concentration $0.33\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{NADH} = v_8 - v_{12} - v_{15} \tag{60}$$

6.13 Species PEP

Name Phosphoenolpyruvate

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

This species takes part in two reactions (as a reactant in vPK and as a product in vlpPEP).

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

6.14 Species Pyr

Name Pyruvate

Initial concentration $8.7\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

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

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

6.15 Species ACA

Name Acetaldehyde

Initial concentration $1.48153\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ACA} = v_{11} - v_{12} - 59v_{18} \tag{63}$$

6.16 Species EtOH

Initial concentration $19.2379\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in vdifEtOH and as a product in vADH).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{EtOH} = v_{12} - 59v_{13} \tag{64}$$

6.17 Species EtOHX

Name Extracellular ethanol

Initial concentration $16.4514\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in voutEtOH and as a product in vdifEtOH).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{EtOHX} = v_{13} - v_{14} \tag{65}$$

6.18 Species Glyc

Name Glycerol

Initial concentration $4.196\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in vdifGlyc and as a product in vlpGlyc).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Glyc} = v_{15} - 59v_{16} \tag{66}$$

6.19 Species GlycX

Name Extracellular glycerol

Initial concentration $1.68478\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in voutGlyc and as a product in vdifGlyc).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{GlycX} = v_{16} - v_{17} \tag{67}$$

6.20 Species ACAX

Name Extracellular acetaldehyde

Initial concentration $1.28836\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in three reactions (as a reactant in voutACA, vlacto and as a product in vdifACA).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ACAX} = v_{18} - v_{19} - v_{20} \tag{68}$$

6.21 Species CNX

Name Extracellular cyanide

Initial concentration $5.20358\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in vlacto and as a product in vinCN).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{CNX} = v_{21} - v_{20} \tag{69}$$

6.22 Species AMP

Name AMP

Initial concentration $0.33\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in vAK and as a modifier in vPFK).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{AMP} = -v_{24} \tag{70}$$

6.23 Species P

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

This species takes part in four reactions (as a product in voutEtOH, voutGlyc, voutACA, vlacto), which do not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{P} = 0 \tag{71}$$

6.24 Species CNX0

Name Mixed flow cyanide

Initial concentration $5.6\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{CNX0} = 0 \tag{72}$$

6.25 Species GlcX0

Name Mixed flow glucose

Initial concentration $24\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{GlcX0} = 0 \tag{73}$$

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