SBML Model Report

Model name: "Holzhutter2004_Erythrocyte_Metabolism"

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 September seventh 2006 at 3:04 p. m. and last time modified at April eighth 2016 at 3:29 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	1
species types	0	species	45
events	0	constraints	0
reactions	38	function definitions	0
global parameters	0	unit definitions	6
rules	0	initial assignments	0

Model Notes

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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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Biomodels CurationThe model simulates the flux values as given for „kinetic model„ in Table 1 of the paper. The model was successfully tested on Jarnac.

2 Unit Definitions

This is an overview of nine 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 hour

Definition 3600 s

2.3 Unit `mM`

Name mM

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

2.4 Unit `mM_per_hour`

Name mM_per_hour

Definition $\mathrm{mmol} \cdot \mathrm{l}^{-1} \cdot (3600\ \mathrm{s})^{-1}$

2.5 Unit `hour_inverse`

Name hour_inverse

Definition $(3600\ \mathrm{s})^{-1}$

2.6 Unit per_mM_hour

Name per_mM_hour

Definition $\mathrm{mmol}^{-1} \cdot 1 \cdot (3600\ \mathrm{s})^{-1}$

2.7 Unit volume

Notes Litre is the predefined SBML unit for volume.

Definition l

2.8 Unit area

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

Definition m^2

2.9 Unit length

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

Definition m

3 Compartment

This model contains one compartment.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
compartment	cytoplasm		3	1	litre	☑	

3.1 Compartment compartment

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

Name cytoplasm

4 Species

This model contains 45 species. The boundary condition of five 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
`Glcin`	Glucose in	`compartment`	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
`MgATP`	MgATP	`compartment`	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
`Glc6P`	Glucose 6-phosphate	`compartment`	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
`MgADP`	MgADP	`compartment`	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
`Fru6P`	Fructose 6-phosphate	`compartment`	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
`Fru16P2`	Fructose 1,6-phosphate	`compartment`	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
`GraP`	Glyceraldehyde 3-phosphate	`compartment`	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
`DHAP`	Dihydroxyacetone phosphate	`compartment`	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
`Phi`	Phosphate	`compartment`	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
`NAD`	NAD	`compartment`	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
`Gri13P2`	1,3-Bisphospho-D-glycerate	`compartment`	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
`NADH`	NADH	`compartment`	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
`Gri3P`	3-Phospho-D-glycerate	`compartment`	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
`Gri23P2f`	2,3-Bisphospho-D-glycerate	`compartment`	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
`Gri2P`	2-Phospho-D-glycerate	`compartment`	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
`PEP`	Phosphoenolpyruvate	`compartment`	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
`Pyr`	Pyruvate	`compartment`	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
`Lac`	Lactate	`compartment`	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
`NADPHf`	NADPH	`compartment`	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
`NADPf`	NADP	`compartment`	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
`AMPf`	AMP	`compartment`	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟

Id	Name	Compartment	Derived Unit	Constant	Boundary Condition
ADPf	ADP	compartment	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
GlcA6P	Phospho-D-glucono-1,5-lactone	compartment	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Rul5P	Ribulose 5-phosphate	compartment	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
GSSG	Oxidized Glutathione	compartment	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
GSH	Reduced Glutathione	compartment	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Xul5P	Xylulose 5-phosphate	compartment	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Rib5P	Ribose 5-phosphate	compartment	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Sed7P	Sedoheptulose 7-phosphate	compartment	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
E4P	Erythrose 4-phosphate	compartment	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
MgAMP	MgAMP	compartment	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
ATPf	ATP	compartment	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Mgf	Mg	compartment	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
MgGri23P2	MgGri23P2	compartment	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
P1NADP	Protein1 bound NADP	compartment	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
P1f	Protein1	compartment	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
P1NADPH	Protein1 bound NADPH	compartment	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
P2NADP	Protein2 bound NADP	compartment	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
P2f	Protein2	compartment	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
P2NADPH	Protein2 bound NADPH	compartment	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
PRPP	PRPP	compartment	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	☑
Lacex	External Lactate	compartment	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	☑
Pyrex	External Pyruvate	compartment	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	☑
Glcout	Glucose outside	compartment	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	☑
Phiex	Phosphate external	compartment	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	☑

5 Reactions

This model contains 38 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	vGLT	Glucose transport	$\text{Glcout} \rightleftharpoons \text{Glcin}$	
2	vHEX	Hexokinase	$\text{Glcin} + \text{MgATP} \overset{\text{Mgf, Gri23P2f, MgGri23P2}}{\rightleftharpoons} \text{Glc6P} + \text{MgADP}$	
3	vGPI	Glucosephosphate isomerase	$\text{Glc6P} \rightleftharpoons \text{Fru6P}$	
4	vPFK	Phosphofructokinase	$\text{MgATP} + \text{Fru6P} \overset{\text{ATPf, Mgf, AMPf, MgAMP}}{\rightleftharpoons} \text{Fru16P2} + \text{MgADP}$	
5	vALD	Aldolase	$\text{Fru16P2} \rightleftharpoons \text{GraP} + \text{DHAP}$	
6	vTPI	Triosephosphate isomerase	$\text{DHAP} \rightleftharpoons \text{GraP}$	
7	vGAPDH	Glyceraldehyde 3-phosphate dehydrogenase	$\text{GraP} + \text{Phi} + \text{NAD} \rightleftharpoons \text{NADH} + \text{Gri13P2}$	
8	vPGK	Phosphoglycerate kinase	$\text{MgADP} + \text{Gri13P2} \rightleftharpoons \text{MgATP} + \text{Gri3P}$	
9	vBPGM	Bisphosphoglycerate mutase	$\text{Gri13P2} \overset{\text{MgGri23P2}}{\rightleftharpoons} \text{Gri23P2f}$	
10	vBPGP	Bisphosphoglycerate phosphatase	$\text{Gri23P2f} \overset{\text{MgGri23P2}}{\rightleftharpoons} \text{Gri3P} + \text{Phi}$	
11	vPGM	Phosphoglycerate mutase	$\text{Gri3P} \rightleftharpoons \text{Gri2P}$	
12	vENO	Enolase	$\text{Gri2P} \rightleftharpoons \text{PEP}$	
13	vPK	Pyruvate kinase	$\text{PEP} + \text{MgADP} \overset{\text{ATPf, Fru16P2}}{\rightleftharpoons} \text{MgATP} + \text{Pyr}$	
14	vLDHNADH	Lactate dehydrogenase	$\text{NADH} + \text{Pyr} \rightleftharpoons \text{Lac} + \text{NAD}$	
15	vLDHNADPH	Lactate dehydrogenase	$\text{Pyr} + \text{NADPHf} \rightleftharpoons \text{Lac} + \text{NADPf}$	
16	vATPase	ATPase	$\text{MgATP} \rightleftharpoons \text{Phi} + \text{MgADP}$	
17	vAK	Adenylate kinase	$\text{MgATP} + \text{AMPf} \rightleftharpoons \text{ADPf} + \text{MgADP}$	

№	Id	Name	Reaction Equation	SBO
18	vG6PDH	Glucose 6-phosphate dehydrogenase	$\mathrm{Glc6P} + \mathrm{NADPf} \overset{\text{ATPf, MgATP, Gri23P2f, MgGri23P2}}{\rightleftharpoons} \mathrm{GlcA6P} + \mathrm{NADPHf}$	
19	vPGLDH	Phosphogluconate dehydrogenase	$\mathrm{GlcA6P} + \mathrm{NADPf} \overset{\text{Gri23P2f, MgGri23P2, ATPf, MgATP}}{\rightleftharpoons} \mathrm{Rul5P} + \mathrm{NADPHf}$	
20	vGSSGRD	Glutathione reductase	$\mathrm{GSSG} + \mathrm{NADPHf} \rightleftharpoons 2\,\mathrm{GSH} + \mathrm{NADPf}$	
21	vGSHox	Glutathione oxidation	$2\,\mathrm{GSH} \rightleftharpoons \mathrm{GSSG}$	
22	vRibPepi	Phosphoribulose epimerase	$\mathrm{Rul5P} \rightleftharpoons \mathrm{Xul5P}$	
23	vRibPiso	Ribose phosphate isomerase	$\mathrm{Rul5P} \rightleftharpoons \mathrm{Rib5P}$	
24	vTrKet1	Transketolase 1	$\mathrm{Xul5P} + \mathrm{Rib5P} \rightleftharpoons \mathrm{GraP} + \mathrm{Sed7P}$	
25	vTrAld	Transaldolase	$\mathrm{GraP} + \mathrm{Sed7P} \rightleftharpoons \mathrm{E4P} + \mathrm{Fru6P}$	
26	vPPRPPS	Phosphoribosylpyrophosphate synthetase	$\mathrm{MgATP} + \mathrm{Rib5P} \rightleftharpoons \mathrm{MgAMP} + \mathrm{PRPP}$	
27	vTrKet2	Transketolase 2	$\mathrm{Xul5P} + \mathrm{E4P} \rightleftharpoons \mathrm{GraP} + \mathrm{Fru6P}$	
28	vPhiexch	Phosphate exchange	$\mathrm{Phiex} \rightleftharpoons \mathrm{Phi}$	
29	vLacexch	Lactate exchange	$\mathrm{Lacex} \rightleftharpoons \mathrm{Lac}$	
30	vPyrexch	Pyruvate exchange	$\mathrm{Pyrex} \rightleftharpoons \mathrm{Pyr}$	
31	vMgATP	MgATP dissociation	$\mathrm{MgATP} \rightleftharpoons \mathrm{Mgf} + \mathrm{ATPf}$	
32	vMgADP	MgADP dissociation	$\mathrm{MgADP} \rightleftharpoons \mathrm{Mgf} + \mathrm{ADPf}$	
33	vMgAMP	MgAMP dissociation	$\mathrm{MgAMP} \rightleftharpoons \mathrm{Mgf} + \mathrm{AMPf}$	
34	vMgGri23P2	MgGri23P2 dissociation	$\mathrm{MgGri23P2} \rightleftharpoons \mathrm{Mgf} + \mathrm{Gri23P2f}$	
35	vP1NADP	P1NADP dissociation	$\mathrm{P1NADP} \rightleftharpoons \mathrm{P1f} + \mathrm{NADPf}$	
36	vP1NADPH	P1NADPH dissociation	$\mathrm{P1NADPH} \rightleftharpoons \mathrm{P1f} + \mathrm{NADPHf}$	
37	vP2NADP	P2NADP dissociation	$\mathrm{P2NADP} \rightleftharpoons \mathrm{P2f} + \mathrm{NADPf}$	
38	vP2NADPH	P2NADPH dissociation	$\mathrm{P2NADPH} \rightleftharpoons \mathrm{P2f} + \mathrm{NADPHf}$	

5.1 Reaction vGLT

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

Name Glucose transport

Reaction equation

$$\text{Glcout} \rightleftharpoons \text{Glcin} \tag{1}$$

Reactant

Table 5: Properties of each reactant.

Id	Name	SBO
Glcout	Glucose outside	

Product

Table 6: Properties of each product.

Id	Name	SBO
Glcin	Glucose in	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \text{vol}\left(\text{compartment}\right) \cdot \frac{\frac{\text{Vmaxv0}}{\text{KMoutv0}} \cdot \left([\text{Glcout}] - \frac{[\text{Glcin}]}{\text{Keqv0}}\right)}{1 + \frac{[\text{Glcout}]}{\text{KMoutv0}} + \frac{[\text{Glcin}]}{\text{KMinv0}} + \frac{\frac{\text{alfav0} \cdot [\text{Glcout}] \cdot [\text{Glcin}]}{\text{KMoutv0}}}{\text{KMinv0}}} \tag{2}$$

Table 7: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmaxv0			33.60	$\text{mmol} \cdot \text{l}^{-1} \cdot (3600\ \text{s})^{-1}$	☑
KMoutv0			1.70	$\text{mmol} \cdot \text{l}^{-1}$	☑
Keqv0			1.00	dimensionless	☑
KMinv0			6.90	$\text{mmol} \cdot \text{l}^{-1}$	☑
alfav0			0.54	dimensionless	☑

5.2 Reaction vHEX

This is a reversible reaction of two reactants forming two products influenced by three modifiers.

Name Hexokinase

Reaction equation

$$\mathrm{Glcin} + \mathrm{MgATP} \xrightleftharpoons{\text{Mgf, Gri23P2f, MgGri23P2}} \mathrm{Glc6P} + \mathrm{MgADP} \tag{3}$$

Reactants

Table 8: Properties of each reactant.

Id	Name	SBO
Glcin	Glucose in	
MgATP	MgATP	

Modifiers

Table 9: Properties of each modifier.

Id	Name	SBO
Mgf	Mg	
Gri23P2f	2,3-Bisphospho-D-glycerate	
MgGri23P2	MgGri23P2	

Products

Table 10: Properties of each product.

Id	Name	SBO
Glc6P	Glucose 6-phosphate	
MgADP	MgADP	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \frac{\frac{\mathrm{Inhibv1}\cdot[\mathrm{Glcin}]}{[\mathrm{Glcin}]+\mathrm{KMGlcv1}} \cdot \frac{\mathrm{Vmax1v1}}{\mathrm{KMgATPv1}} \cdot \left([\mathrm{MgATP}] + \frac{\frac{\mathrm{Vmax2v1}}{\mathrm{Vmax1v1}}\cdot[\mathrm{MgATP}]\cdot[\mathrm{Mgf}]}{\mathrm{KMgATPMgv1}} - \frac{[\mathrm{Glc6P}]\cdot[\mathrm{MgADP}]}{\mathrm{Keqv1}}\right)}{1 + \frac{[\mathrm{MgATP}]}{\mathrm{KMgATPv1}} \cdot \left(1 + \frac{[\mathrm{Mgf}]}{\mathrm{KMgATPMgv1}}\right) + \frac{[\mathrm{Mgf}]}{\mathrm{KMgv1}} + \left(1.55 + \frac{[\mathrm{Glc6P}]}{\mathrm{KGlc6Pv1}}\right) \cdot \left(1 + \frac{[\mathrm{Mgf}]}{\mathrm{KMgv1}}\right) + \frac{[\mathrm{Gri23P2f}]+[\mathrm{MgGri23P2}]}{\mathrm{K23P2Gv1}} + \frac{[\mathrm{Mgf}]\cdot(}{\mathrm{K}}} \tag{4}$$

Table 11: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Inhibv1			1.000	dimensionless	☑
KMGlcv1			0.100	$\mathrm{mmol}\cdot\mathrm{l}^{-1}$	☑
Vmax1v1			15.800	$\mathrm{mmol}\cdot\mathrm{l}^{-1}\cdot(3600\,\mathrm{s})^{-1}$	☑
KMgATPv1			1.440	$\mathrm{mmol}\cdot\mathrm{l}^{-1}$	☑
Vmax2v1			33.200	$\mathrm{mmol}\cdot\mathrm{l}^{-1}\cdot(3600\,\mathrm{s})^{-1}$	☑
KMgATPMgv1			1.140	$\mathrm{mmol}\cdot\mathrm{l}^{-1}$	☑
Keqv1			3900.000	$\mathrm{mmol}\cdot\mathrm{l}^{-1}$	☑
KMgv1			1.030	$\mathrm{mmol}\cdot\mathrm{l}^{-1}$	☑
KGlc6Pv1			0.005	$\mathrm{mmol}\cdot\mathrm{l}^{-1}$	☑
K23P2Gv1			2.700	$\mathrm{mmol}\cdot\mathrm{l}^{-1}$	☑
KMg23P2Gv1			3.440	$\mathrm{mmol}\cdot\mathrm{l}^{-1}$	☑

5.3 Reaction vGPI

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

Name Glucosephosphate isomerase

Reaction equation

$$\mathrm{Glc6P} \rightleftharpoons \mathrm{Fru6P} \tag{5}$$

Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
Glc6P	Glucose 6-phosphate	

Product

Table 13: Properties of each product.

Id	Name	SBO
Fru6P	Fructose 6-phosphate	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \frac{\mathrm{Vmaxv2} \cdot \left([\mathrm{Glc6P}] - \frac{[\mathrm{Fru6P}]}{\mathrm{Keqv2}}\right)}{[\mathrm{Glc6P}] + \mathrm{KGlc6Pv2} \cdot \left(1 + \frac{[\mathrm{Fru6P}]}{\mathrm{KFru6Pv2}}\right)} \tag{6}$$

Table 14: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmaxv2			935.000	$\mathrm{mmol} \cdot \mathrm{l}^{-1} \cdot (3600\ \mathrm{s})^{-1}$	☑
Keqv2			0.393	dimensionless	☑
KGlc6Pv2			0.182	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KFru6Pv2			0.071	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑

5.4 Reaction vPFK

This is a reversible reaction of two reactants forming two products influenced by four modifiers.

Name Phosphofructokinase

Reaction equation

$$\mathrm{MgATP} + \mathrm{Fru6P} \xrightleftharpoons{\text{ATPf, Mgf, AMPf, MgAMP}} \mathrm{Fru16P2} + \mathrm{MgADP} \tag{7}$$

Reactants

Table 15: Properties of each reactant.

Id	Name	SBO
MgATP	MgATP	
Fru6P	Fructose 6-phosphate	

Modifiers

Table 16: Properties of each modifier.

Id	Name	SBO
ATPf	ATP	
Mgf	Mg	
AMPf	AMP	
MgAMP	MgAMP	

Products

Table 17: Properties of each product.

Id	Name	SBO
Fru16P2	Fructose 1,6-phosphate	
MgADP	MgADP	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \frac{\mathrm{Vmaxv3} \cdot \left([\mathrm{Fru6P}] \cdot [\mathrm{MgATP}] - \frac{[\mathrm{Fru16P2}] \cdot [\mathrm{MgADP}]}{\mathrm{Keqv3}}\right)}{([\mathrm{Fru6P}] + \mathrm{KFru6Pv3}) \cdot ([\mathrm{MgATP}] + \mathrm{KMgATPv3}) \cdot \left(1 + \mathrm{L0v3} \cdot \left(\frac{\left(1+\frac{[\mathrm{ATPf}]}{\mathrm{KATPv3}}\right) \cdot \left(1+\frac{[\mathrm{Mgf}]}{\mathrm{KMgv3}}\right)}{\left(1+\frac{[\mathrm{AMPf}]+[\mathrm{MgAMP}]}{\mathrm{KAMPv3}}\right) \cdot \left(1+\frac{[\mathrm{Fru6P}]}{\mathrm{KFru6Pv3}}\right)}\right)^4\right)} \tag{8}$$

Table 18: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmaxv3			239.000	$\mathrm{mmol} \cdot \mathrm{l}^{-1} \cdot (3600\ \mathrm{s})^{-1}$	☑
Keqv3			100000.000	dimensionless	☑
KFru6Pv3			0.100	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KMgATPv3			0.068	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
L0v3			0.001	dimensionless	☑
KATPv3			0.010	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KMgv3			0.440	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KAMPv3			0.033	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑

5.5 Reaction vALD

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

Name Aldolase

Reaction equation

$$\mathrm{Fru16P2} \rightleftharpoons \mathrm{GraP} + \mathrm{DHAP} \tag{9}$$

Reactant

Table 19: Properties of each reactant.

Id	Name	SBO
Fru16P2	Fructose 1,6-phosphate	

Products

Table 20: Properties of each product.

Id	Name	SBO
GraP	Glyceraldehyde 3-phosphate	
DHAP	Dihydroxyacetone phosphate	

Kinetic Law

Derived unit contains undeclared units

$$\begin{aligned} v_5 &= \mathrm{vol}\,(\mathrm{compartment}) \\ &\cdot \frac{\frac{\mathrm{Vmaxv4}}{\mathrm{KFru16P2v4}} \cdot \left([\mathrm{Fru16P2}] - \frac{[\mathrm{GraP}]\cdot[\mathrm{DHAP}]}{\mathrm{Keqv4}}\right)}{1 + \frac{[\mathrm{Fru16P2}]}{\mathrm{KFru16P2v4}} + \frac{[\mathrm{GraP}]}{\mathrm{KiGraPv4}} + \frac{[\mathrm{DHAP}]\cdot([\mathrm{GraP}]+\mathrm{KGraPv4})}{\mathrm{KDHAPv4}\cdot\mathrm{KiGraPv4}} + \frac{[\mathrm{Fru16P2}]\cdot[\mathrm{GraP}]}{\mathrm{KFru16P2v4}\cdot\mathrm{KiiGraPv4}}} \end{aligned} \tag{10}$$

Table 21: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmaxv4			98.910	$\mathrm{mmol}\cdot\mathrm{l}^{-1}\cdot(3600\ \mathrm{s})^{-1}$	☑
KFru16P2v4			0.007	$\mathrm{mmol}\cdot\mathrm{l}^{-1}$	☑

Id	Name	SBO	Value	Unit	Constant
Keqv4			0.114	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KiGraPv4			0.057	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KGraPv4			0.191	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KDHAPv4			0.036	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KiiGraPv4			0.176	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑

5.6 Reaction vTPI

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

Name Triosephosphate isomerase

Reaction equation

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

Reactant

Table 22: Properties of each reactant.

Id	Name	SBO
DHAP	Dihydroxyacetone phosphate	

Product

Table 23: Properties of each product.

Id	Name	SBO
GraP	Glyceraldehyde 3-phosphate	

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \frac{\mathrm{Vmaxv5} \cdot \left([\mathrm{DHAP}] - \frac{[\mathrm{GraP}]}{\mathrm{Keqv5}}\right)}{[\mathrm{DHAP}] + \mathrm{KDHAPv5} \cdot \left(1 + \frac{[\mathrm{GraP}]}{\mathrm{KGraPv5}}\right)} \tag{12}$$

Table 24: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmaxv5			5456.600	$\text{mmol} \cdot \text{l}^{-1} \cdot (3600\ \text{s})^{-1}$	☑
Keqv5			0.041	dimensionless	☑
KDHAPv5			0.838	$\text{mmol} \cdot \text{l}^{-1}$	☑
KGraPv5			0.428	$\text{mmol} \cdot \text{l}^{-1}$	☑

5.7 Reaction vGAPDH

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

Name Glyceraldehyde 3-phosphate dehydrogenase

Reaction equation

$$\text{GraP} + \text{Phi} + \text{NAD} \rightleftharpoons \text{NADH} + \text{Gri13P2} \tag{13}$$

Reactants

Table 25: Properties of each reactant.

Id	Name	SBO
GraP	Glyceraldehyde 3-phosphate	
Phi	Phosphate	
NAD	NAD	

Products

Table 26: Properties of each product.

Id	Name	SBO
NADH	NADH	
Gri13P2	1,3-Bisphospho-D-glycerate	

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \frac{\frac{\mathrm{Vmaxv6}}{\mathrm{KNADv6}\cdot\mathrm{KGraPv6}\cdot\mathrm{KPv6}} \cdot \left([\mathrm{NAD}]\cdot[\mathrm{GraP}]\cdot[\mathrm{Phi}] - \frac{[\mathrm{Gri13P2}]\cdot[\mathrm{NADH}]}{\mathrm{Keqv6}}\right)}{\left(1+\frac{[\mathrm{NAD}]}{\mathrm{KNADv6}}\right)\cdot\left(1+\frac{[\mathrm{GraP}]}{\mathrm{KGraPv6}}\right)\cdot\left(1+\frac{[\mathrm{Phi}]}{\mathrm{KPv6}}\right) + \left(1+\frac{[\mathrm{NADH}]}{\mathrm{KNADHv6}}\right)\cdot\left(1+\frac{[\mathrm{Gri13P2}]}{\mathrm{K13P2Gv6}}\right) - 1} \tag{14}$$

Table 27: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmaxv6			4300.000	$\mathrm{mmol}\cdot\mathrm{l}^{-1}\cdot(3600\ \mathrm{s})^{-1}$	☑
KNADv6			0.050	$\mathrm{mmol}\cdot\mathrm{l}^{-1}$	☑
KGraPv6			0.005	$\mathrm{mmol}\cdot\mathrm{l}^{-1}$	☑
KPv6			3.900	$\mathrm{mmol}\cdot\mathrm{l}^{-1}$	☑
Keqv6			$1.92\cdot10^{-4}$	dimensionless	☑
KNADHv6			0.008	$\mathrm{mmol}\cdot\mathrm{l}^{-1}$	☑
K13P2Gv6			0.004	$\mathrm{mmol}\cdot\mathrm{l}^{-1}$	☑

5.8 Reaction vPGK

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

Name Phosphoglycerate kinase

Reaction equation

$$\mathrm{MgADP} + \mathrm{Gri13P2} \rightleftharpoons \mathrm{MgATP} + \mathrm{Gri3P} \tag{15}$$

Reactants

Table 28: Properties of each reactant.

Id	Name	SBO
MgADP	MgADP	
Gri13P2	1,3-Bisphospho-D-glycerate	

Products

Table 29: Properties of each product.

Id	Name	SBO
MgATP	MgATP	
Gri3P	3-Phospho-D-glycerate	

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \frac{\frac{\mathrm{Vmaxv7}}{\mathrm{KMgADPv7}\cdot\mathrm{K13P2Gv7}} \cdot \left([\mathrm{MgADP}]\cdot[\mathrm{Gri13P2}] - \frac{[\mathrm{MgATP}]\cdot[\mathrm{Gri3P}]}{\mathrm{Keqv7}}\right)}{\left(1+\frac{[\mathrm{MgADP}]}{\mathrm{KMgADPv7}}\right)\cdot\left(1+\frac{[\mathrm{Gri13P2}]}{\mathrm{K13P2Gv7}}\right)+\left(1+\frac{[\mathrm{MgATP}]}{\mathrm{KMgATPv7}}\right)\cdot\left(1+\frac{[\mathrm{Gri3P}]}{\mathrm{K3PGv7}}\right)-1} \tag{16}$$

Table 30: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmaxv7			5000.000	$\mathrm{mmol}\cdot\mathrm{l}^{-1}\cdot(3600\ \mathrm{s})^{-1}$	☑
KMgADPv7			0.350	$\mathrm{mmol}\cdot\mathrm{l}^{-1}$	☑
K13P2Gv7			0.002	$\mathrm{mmol}\cdot\mathrm{l}^{-1}$	☑
Keqv7			1455.000	dimensionless	☑
KMgATPv7			0.480	$\mathrm{mmol}\cdot\mathrm{l}^{-1}$	☑
K3PGv7			1.200	$\mathrm{mmol}\cdot\mathrm{l}^{-1}$	☑

5.9 Reaction vBPGM

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

Name Bisphosphoglycerate mutase

Reaction equation

$$\mathrm{Gri13P2} \xrightleftharpoons{\mathrm{MgGri23P2}} \mathrm{Gri23P2f} \tag{17}$$

Reactant

Table 31: Properties of each reactant.

Id	Name	SBO
Gri13P2	1,3-Bisphospho-D-glycerate	

Modifier

Table 32: Properties of each modifier.

Id	Name	SBO
MgGri23P2	MgGri23P2	

Product

Table 33: Properties of each product.

Id	Name	SBO
Gri23P2f	2,3-Bisphospho-D-glycerate	

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \mathrm{vol}\left(\mathrm{compartment}\right) \cdot \frac{\mathrm{kDPGMv8} \cdot \left(\left[\mathrm{Gri13P2}\right] - \frac{\left[\mathrm{Gri23P2f}\right]+\left[\mathrm{MgGri23P2}\right]}{\mathrm{Keqv8}}\right)}{1 + \frac{\left[\mathrm{Gri23P2f}\right]+\left[\mathrm{MgGri23P2}\right]}{\mathrm{K23P2Gv8}}} \tag{18}$$

Table 34: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
kDPGMv8			76000.00	$(3600\ \mathrm{s})^{-1}$	☑
Keqv8			100000.00	dimensionless	☑
K23P2Gv8			0.04	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑

5.10 Reaction vBPGP

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

Name Bisphosphoglycerate phosphatase

Reaction equation

$$\text{Gri23P2f} \xrightleftharpoons{\text{MgGri23P2}} \text{Gri3P} + \text{Phi} \tag{19}$$

Reactant

Table 35: Properties of each reactant.

Id	Name	SBO
Gri23P2f	2,3-Bisphospho-D-glycerate	

Modifier

Table 36: Properties of each modifier.

Id	Name	SBO
MgGri23P2	MgGri23P2	

Products

Table 37: Properties of each product.

Id	Name	SBO
Gri3P	3-Phospho-D-glycerate	
Phi	Phosphate	

Kinetic Law

Derived unit $0.0010\ \text{mol} \cdot (3600\ \text{s})^{-1}$

$$v_{10} = \text{vol}\,(\text{compartment}) \cdot \frac{\text{Vmaxv9} \cdot \left([\text{Gri23P2f}] + [\text{MgGri23P2}] - \frac{[\text{Gri3P}]}{\text{Keqv9}}\right)}{[\text{Gri23P2f}] + [\text{MgGri23P2}] + \text{K23P2Gv9}} \tag{20}$$

Table 38: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmaxv9			0.53	$\text{mmol} \cdot \text{l}^{-1} \cdot (3600\ \text{s})^{-1}$	☑
Keqv9			100000.00	dimensionless	☑
K23P2Gv9			0.20	$\text{mmol} \cdot \text{l}^{-1}$	☑

5.11 Reaction vPGM

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

Name Phosphoglycerate mutase

Reaction equation

$$\text{Gri3P} \rightleftharpoons \text{Gri2P} \tag{21}$$

Reactant

Table 39: Properties of each reactant.

Id	Name	SBO
Gri3P	3-Phospho-D-glycerate	

Product

Table 40: Properties of each product.

Id	Name	SBO
Gri2P	2-Phospho-D-glycerate	

Kinetic Law

Derived unit contains undeclared units

$$v_{11} = \text{vol}(\text{compartment}) \cdot \frac{\text{Vmaxv10} \cdot \left([\text{Gri3P}] - \frac{[\text{Gri2P}]}{\text{Keqv10}}\right)}{[\text{Gri3P}] + \text{K3PGv10} \cdot \left(1 + \frac{[\text{Gri2P}]}{\text{K2PGv10}}\right)} \tag{22}$$

Table 41: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmaxv10			2000.000	$\text{mmol} \cdot \text{l}^{-1} \cdot (3600\ \text{s})^{-1}$	☑
Keqv10			0.145	dimensionless	☑
K3PGv10			5.000	$\text{mmol} \cdot \text{l}^{-1}$	☑
K2PGv10			1.000	$\text{mmol} \cdot \text{l}^{-1}$	☑

5.12 Reaction vENO

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

Name Enolase

Reaction equation

$$\text{Gri2P} \rightleftharpoons \text{PEP} \tag{23}$$

Reactant

Table 42: Properties of each reactant.

Id	Name	SBO
Gri2P	2-Phospho-D-glycerate	

Product

Table 43: Properties of each product.

Id	Name	SBO
PEP	Phosphoenolpyruvate	

Kinetic Law

Derived unit contains undeclared units

$$v_{12} = \text{vol}(\text{compartment}) \cdot \frac{\text{Vmaxv11} \cdot \left([\text{Gri2P}] - \frac{[\text{PEP}]}{\text{Keqv11}}\right)}{[\text{Gri2P}] + \text{K2PGv11} \cdot \left(1 + \frac{[\text{PEP}]}{\text{KPEPv11}}\right)} \tag{24}$$

Table 44: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmaxv11			1500.0	$\text{mmol} \cdot \text{l}^{-1} \cdot (3600\ \text{s})^{-1}$	☑
Keqv11			1.7	dimensionless	☑
K2PGv11			1.0	$\text{mmol} \cdot \text{l}^{-1}$	☑
KPEPv11			1.0	$\text{mmol} \cdot \text{l}^{-1}$	☑

5.13 Reaction vPK

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

Name Pyruvate kinase

Reaction equation

$$\mathrm{PEP} + \mathrm{MgADP} \overset{\mathrm{ATPf,\ Fru16P2}}{\rightleftharpoons} \mathrm{MgATP} + \mathrm{Pyr} \tag{25}$$

Reactants

Table 45: Properties of each reactant.

Id	Name	SBO
PEP	Phosphoenolpyruvate	
MgADP	MgADP	

Modifiers

Table 46: Properties of each modifier.

Id	Name	SBO
ATPf	ATP	
Fru16P2	Fructose 1,6-phosphate	

Products

Table 47: Properties of each product.

Id	Name	SBO
MgATP	MgATP	
Pyr	Pyruvate	

Kinetic Law

Derived unit contains undeclared units

$$v_{13} = \mathrm{vol}\,(\mathrm{compartment}) \cdot \frac{\mathrm{Vmaxv12} \cdot \left([\mathrm{PEP}] \cdot [\mathrm{MgADP}] - \frac{[\mathrm{Pyr}] \cdot [\mathrm{MgATP}]}{\mathrm{Keqv12}}\right)}{([\mathrm{PEP}] + \mathrm{KPEPv12}) \cdot ([\mathrm{MgADP}] + \mathrm{KMgADPv12}) \cdot \left(1 + \frac{\mathrm{L0v12} \cdot \left(1 + \frac{[\mathrm{ATPf}] + [\mathrm{MgATP}]}{\mathrm{KATPv12}}\right)^4}{\left(1 + \frac{[\mathrm{PEP}]}{\mathrm{KPEPv12}}\right)^4 \cdot \left(1 + \frac{[\mathrm{Fru16P2}]}{\mathrm{KFru16P2v12}}\right)^4}\right)} \tag{26}$$

Table 48: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
`Vmaxv12`			570.000	$\mathrm{mmol} \cdot \mathrm{l}^{-1} \cdot (3600\ \mathrm{s})^{-1}$	☑
`Keqv12`			13790.000	dimensionless	☑
`KPEPv12`			0.225	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
`KMgADPv12`			0.474	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
`L0v12`			19.000	dimensionless	☑
`KATPv12`			3.390	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
`KFru16P2v12`			0.005	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑

5.14 Reaction `vLDHNADH`

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

Name Lactate dehydrogenase

Reaction equation

$$\mathrm{NADH} + \mathrm{Pyr} \rightleftharpoons \mathrm{Lac} + \mathrm{NAD} \tag{27}$$

Reactants

Table 49: Properties of each reactant.

Id	Name	SBO
`NADH`	NADH	
`Pyr`	Pyruvate	

Products

Table 50: Properties of each product.

Id	Name	SBO
Lac	Lactate	
NAD	NAD	

Kinetic Law

Derived unit $0.0010\ \mathrm{mol} \cdot (3600\ \mathrm{s})^{-1}$

$$v_{14} = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{Vmaxv13} \cdot \left([\mathrm{Pyr}] \cdot [\mathrm{NADH}] - \frac{[\mathrm{Lac}] \cdot [\mathrm{NAD}]}{\mathrm{Keqv13}} \right) \tag{28}$$

Table 51: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmaxv13			2800000.0	$\mathrm{mmol}^{-1} \cdot 1 \cdot (3600\ \mathrm{s})^{-1}$	☑
Keqv13			9090.0	dimensionless	☑

5.15 Reaction vLDHNADPH

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

Name Lactate dehydrogenase

Reaction equation

$$\mathrm{Pyr} + \mathrm{NADPHf} \rightleftharpoons \mathrm{Lac} + \mathrm{NADPf} \tag{29}$$

Reactants

Table 52: Properties of each reactant.

Id	Name	SBO
Pyr	Pyruvate	
NADPHf	NADPH	

Products

Table 53: Properties of each product.

Id	Name	SBO
Lac	Lactate	
NADPf	NADP	

Kinetic Law

Derived unit $0.0010\ \mathrm{mol} \cdot (3600\ \mathrm{s})^{-1}$

$$v_{15} = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{kLDHv14} \cdot \left([\mathrm{Pyr}] \cdot [\mathrm{NADPHf}] - \frac{[\mathrm{Lac}] \cdot [\mathrm{NADPf}]}{\mathrm{Keqv14}} \right) \tag{30}$$

Table 54: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
kLDHv14			243.4	$\mathrm{mmol}^{-1} \cdot \mathrm{l} \cdot (3600\ \mathrm{s})^{-1}$	☑
Keqv14			14181.8	dimensionless	☑

5.16 Reaction vATPase

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

Name ATPase

Reaction equation

$$\mathrm{MgATP} \rightleftharpoons \mathrm{Phi} + \mathrm{MgADP} \tag{31}$$

Reactant

Table 55: Properties of each reactant.

Id	Name	SBO
MgATP	MgATP	

Products

Table 56: Properties of each product.

Id	Name	SBO
Phi	Phosphate	
MgADP	MgADP	

Kinetic Law

Derived unit $(3600\ \mathrm{s})^{-1} \cdot \mathrm{mmol}$

$$v_{16} = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{kATPasev15} \cdot [\mathrm{MgATP}] \tag{32}$$

Table 57: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
kATPasev15			1.68	$(3600\ \mathrm{s})^{-1}$	☑

5.17 Reaction vAK

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

Name Adenylate kinase

Reaction equation

$$\mathrm{MgATP} + \mathrm{AMPf} \rightleftharpoons \mathrm{ADPf} + \mathrm{MgADP} \tag{33}$$

Reactants

Table 58: Properties of each reactant.

Id	Name	SBO
MgATP	MgATP	
AMPf	AMP	

Products

Table 59: Properties of each product.

Id	Name	SBO
ADPf	ADP	

Id	Name	SBO
MgADP	MgADP	

Kinetic Law

Derived unit contains undeclared units

$$v_{17} = \mathrm{vol}\,(\mathrm{compartment}) \cdot \frac{\frac{\mathrm{Vmaxv16}}{\mathrm{KATPv16 \cdot KAMPv16}} \cdot \left([\mathrm{MgATP}] \cdot [\mathrm{AMPf}] - \frac{[\mathrm{MgADP}] \cdot [\mathrm{ADPf}]}{\mathrm{Keqv16}}\right)}{\left(1 + \frac{[\mathrm{MgATP}]}{\mathrm{KATPv16}}\right) \cdot \left(1 + \frac{[\mathrm{AMPf}]}{\mathrm{KAMPv16}}\right) + \frac{[\mathrm{MgADP}] + [\mathrm{ADPf}]}{\mathrm{KADPv16}} + \frac{[\mathrm{MgADP}] \cdot [\mathrm{ADPf}]}{\mathrm{KADPv16}^2}} \tag{34}$$

Table 60: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmaxv16			1380.00	$\mathrm{mmol} \cdot \mathrm{l}^{-1} \cdot (3600\ \mathrm{s})^{-1}$	☑
KATPv16			0.09	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KAMPv16			0.08	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
Keqv16			0.25	dimensionless	☑
KADPv16			0.11	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑

5.18 Reaction vG6PDH

This is a reversible reaction of two reactants forming two products influenced by four modifiers.

Name Glucose 6-phosphate dehydrogenase

Reaction equation

$$\mathrm{Glc6P} + \mathrm{NADPf} \xrightleftharpoons{\text{ATPf, MgATP, Gri23P2f, MgGri23P2}} \mathrm{GlcA6P} + \mathrm{NADPHf} \tag{35}$$

Reactants

Table 61: Properties of each reactant.

Id	Name	SBO
Glc6P	Glucose 6-phosphate	
NADPf	NADP	

Modifiers

Table 62: Properties of each modifier.

Id	Name	SBO
ATPf	ATP	
MgATP	MgATP	
Gri23P2f	2,3-Bisphospho-D-glycerate	
MgGri23P2	MgGri23P2	

Products

Table 63: Properties of each product.

Id	Name	SBO
GlcA6P	Phospho-D-glucono-1,5-lactone	
NADPHf	NADPH	

Kinetic Law

Derived unit contains undeclared units

$$v_{18} = \mathrm{vol}\,(\mathrm{compartment}) \cdot \frac{\frac{\frac{\mathrm{Vmaxv17}}{\mathrm{KG6Pv17}}}{\mathrm{KNADPv17}} \cdot \left([\mathrm{Glc6P}] \cdot [\mathrm{NADPf}] - \frac{[\mathrm{GlcA6P}] \cdot [\mathrm{NADPHf}]}{\mathrm{Keqv17}}\right)}{1 + \frac{[\mathrm{NADPf}] \cdot \left(1 + \frac{[\mathrm{Glc6P}]}{\mathrm{KG6Pv17}}\right)}{\mathrm{KNADPv17}} + \frac{[\mathrm{ATPf}] + [\mathrm{MgATP}]}{\mathrm{KATPv17}} + \frac{[\mathrm{NADPHf}]}{\mathrm{KNADPHv17}} + \frac{[\mathrm{Gri23P2f}] + [\mathrm{MgGri23P2}]}{\mathrm{KPGA23v17}}} \tag{36}$$

Table 64: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmaxv17			162.000	$\mathrm{mmol} \cdot \mathrm{l}^{-1} \cdot (3600\ \mathrm{s})^{-1}$	☑
KG6Pv17			0.067	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KNADPv17			0.004	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
Keqv17			2000.000	dimensionless	☑
KATPv17			0.749	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KNADPHv17			0.003	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KPGA23v17			2.289	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑

5.19 Reaction vPGLDH

This is a reversible reaction of two reactants forming two products influenced by four modifiers.

Name Phosphogluconate dehydrogenase

Reaction equation

$$\mathrm{GlcA6P} + \mathrm{NADPf} \xrightleftharpoons{\text{Gri23P2f, MgGri23P2, ATPf, MgATP}} \mathrm{Rul5P} + \mathrm{NADPHf} \qquad (37)$$

Reactants

Table 65: Properties of each reactant.

Id	Name	SBO
GlcA6P	Phospho-D-glucono-1,5-lactone	
NADPf	NADP	

Modifiers

Table 66: Properties of each modifier.

Id	Name	SBO
Gri23P2f	2,3-Bisphospho-D-glycerate	
MgGri23P2	MgGri23P2	
ATPf	ATP	
MgATP	MgATP	

Products

Table 67: Properties of each product.

Id	Name	SBO
Rul5P	Ribulose 5-phosphate	
NADPHf	NADPH	

Kinetic Law

Derived unit contains undeclared units

$$v_{19} = \mathrm{vol}\,(\mathrm{compartment}) \cdot \frac{\frac{\mathrm{Vmaxv18}}{\mathrm{K6PG1v18}} \cdot \left([\mathrm{GlcA6P}] \cdot [\mathrm{NADPf}] - \frac{[\mathrm{Rul5P}] \cdot [\mathrm{NADPHf}]}{\mathrm{Keqv18}}\right)}{\left(1 + \frac{[\mathrm{NADPf}]}{\mathrm{KNADPv18}}\right) \cdot \left(1 + \frac{[\mathrm{GlcA6P}]}{\mathrm{K6PG1v18}} + \frac{[\mathrm{Gri23P2f}] + [\mathrm{MgGri23P2}]}{\mathrm{KPGA23v18}}\right) + \frac{[\mathrm{ATPf}] + [\mathrm{MgATP}]}{\mathrm{KATPv18}} + \frac{[\mathrm{NADPHf}] \cdot \left(1 + \frac{[\mathrm{GlcA6P}]}{\mathrm{K6PG2v18}}\right)}{\mathrm{KNADPHv18}}} \tag{38}$$

Table 68: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmaxv18			1575.000	$\mathrm{mmol} \cdot \mathrm{l}^{-1} \cdot (3600\ \mathrm{s})^{-1}$	☑
K6PG1v18			0.010	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KNADPv18			0.018	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
Keqv18			141.700	dimensionless	☑
KPGA23v18			0.120	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KATPv18			0.154	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
K6PG2v18			0.058	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KNADPHv18			0.005	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑

5.20 Reaction vGSSGRD

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

Name Glutathione reductase

Reaction equation

$$\mathrm{GSSG} + \mathrm{NADPHf} \rightleftharpoons 2\,\mathrm{GSH} + \mathrm{NADPf} \tag{39}$$

Reactants

Table 69: Properties of each reactant.

Id	Name	SBO
GSSG	Oxidized Glutathione	
NADPHf	NADPH	

Products

Table 70: Properties of each product.

Id	Name	SBO
GSH	Reduced Glutathione	
NADPf	NADP	

Kinetic Law

Derived unit contains undeclared units

$$v_{20} = \mathrm{vol}\left(\mathrm{compartment}\right) \cdot \frac{\mathrm{Vmaxv19} \cdot \left(\frac{[\mathrm{GSSG}] \cdot [\mathrm{NADPHf}]}{\mathrm{KGSSGv19} \cdot \mathrm{KNADPHv19}} - \frac{\frac{[\mathrm{GSH}]^2}{\mathrm{KGSHv19}^2} \cdot [\mathrm{NADPf}]}{\mathrm{KNADPv19} \cdot \mathrm{Keqv19}} \right)}{1 + \frac{[\mathrm{NADPHf}] \cdot \left(1 + \frac{[\mathrm{GSSG}]}{\mathrm{KGSSGv19}}\right)}{\mathrm{KNADPHv19}} + \frac{[\mathrm{NADPf}]}{\mathrm{KNADPv19}} \cdot \left(1 + \frac{[\mathrm{GSH}] \cdot \left(1 + \frac{[\mathrm{GSH}]}{\mathrm{KGSHv19}}\right)}{\mathrm{KGSHv19}}\right)} \tag{40}$$

Table 71: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmaxv19			90.000	$\mathrm{mmol} \cdot \mathrm{l}^{-1} \cdot (3600\ \mathrm{s})^{-1}$	☑
KGSSGv19			0.065	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KNADPHv19			0.009	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KGSHv19			20.000	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KNADPv19			0.070	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
Keqv19			1.040	dimensionless	☑

5.21 Reaction vGSHox

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

Name Glutathione oxidation

Reaction equation

$$2\,\mathrm{GSH} \rightleftharpoons \mathrm{GSSG} \tag{41}$$

Reactant

Table 72: Properties of each reactant.

Id	Name	SBO
GSH	Reduced Glutathione	

Product

Table 73: Properties of each product.

Id	Name	SBO
GSSG	Oxidized Glutathione	

Kinetic Law

Derived unit $(3600\ \mathrm{s})^{-1} \cdot \mathrm{mmol}$

$$v_{21} = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{Kv20} \cdot [\mathrm{GSH}] \tag{42}$$

Table 74: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Kv20			0.03	$(3600\ \mathrm{s})^{-1}$	☑

5.22 Reaction vRibPepi

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

Name Phosphoribulose epimerase

Reaction equation

$$\mathrm{Rul5P} \rightleftharpoons \mathrm{Xul5P} \tag{43}$$

Reactant

Table 75: Properties of each reactant.

Id	Name	SBO
Rul5P	Ribulose 5-phosphate	

Product

Table 76: Properties of each product.

Id	Name	SBO
Xul5P	Xylulose 5-phosphate	

Kinetic Law

Derived unit contains undeclared units

$$v_{22} = \mathrm{vol}\,(\mathrm{compartment}) \cdot \frac{\mathrm{Vmaxv21} \cdot \left([\mathrm{Rul5P}] - \frac{[\mathrm{Xul5P}]}{\mathrm{Keqv21}}\right)}{[\mathrm{Rul5P}] + \mathrm{KRu5Pv21} \cdot \left(1 + \frac{[\mathrm{Xul5P}]}{\mathrm{KX5Pv21}}\right)} \tag{44}$$

Table 77: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmaxv21			4634.00	$\mathrm{mmol} \cdot \mathrm{l}^{-1} \cdot (3600\ \mathrm{s})^{-1}$	☑
Keqv21			2.70	dimensionless	☑
KRu5Pv21			0.19	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KX5Pv21			0.50	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑

5.23 Reaction vRibPiso

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

Name Ribose phosphate isomerase

Reaction equation

$$\mathrm{Rul5P} \rightleftharpoons \mathrm{Rib5P} \tag{45}$$

Reactant

Table 78: Properties of each reactant.

Id	Name	SBO
Rul5P	Ribulose 5-phosphate	

Product

Table 79: Properties of each product.

Id	Name	SBO
Rib5P	Ribose 5-phosphate	

Kinetic Law

Derived unit contains undeclared units

$$v_{23} = \mathrm{vol}\,(\mathrm{compartment}) \cdot \frac{\mathrm{Vmaxv22} \cdot \left([\mathrm{Rul5P}] - \frac{[\mathrm{Rib5P}]}{\mathrm{Keqv22}}\right)}{[\mathrm{Rul5P}] + \mathrm{KRu5Pv22} \cdot \left(1 + \frac{[\mathrm{Rib5P}]}{\mathrm{KR5Pv22}}\right)} \tag{46}$$

Table 80: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmaxv22			730.00	$\mathrm{mmol} \cdot \mathrm{l}^{-1} \cdot (3600\ \mathrm{s})^{-1}$	☑
Keqv22			3.00	dimensionless	☑
KRu5Pv22			0.78	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KR5Pv22			2.20	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑

5.24 Reaction vTrKet1

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

Name Transketolase 1

Reaction equation

$$\mathrm{Xul5P} + \mathrm{Rib5P} \rightleftharpoons \mathrm{GraP} + \mathrm{Sed7P} \tag{47}$$

Reactants

Table 81: Properties of each reactant.

Id	Name	SBO
Xul5P	Xylulose 5-phosphate	
Rib5P	Ribose 5-phosphate	

Products

Table 82: Properties of each product.

Id	Name	SBO
GraP	Glyceraldehyde 3-phosphate	
Sed7P	Sedoheptulose 7-phosphate	

Kinetic Law

Derived unit $0.0010000000000000013\ \mathrm{mol} \cdot (3600\ \mathrm{s})^{-1}$

$$v_{24} = \mathrm{vol}(\mathrm{compartment}) \cdot \frac{\mathrm{Vmaxv23} \cdot \left([\mathrm{Rib5P}] \cdot [\mathrm{Xul5P}] - \frac{[\mathrm{GraP}] \cdot [\mathrm{Sed7P}]}{\mathrm{Keqv23}}\right)}{(\mathrm{K1v23} + [\mathrm{Rib5P}]) \cdot [\mathrm{Xul5P}] + (\mathrm{K2v23} + \mathrm{K6v23} \cdot [\mathrm{Sed7P}]) \cdot [\mathrm{Rib5P}] + (\mathrm{K3v23} + \mathrm{K5v23} \cdot [\mathrm{Sed7P}]) \cdot [\mathrm{GraP}] +} \quad (48)$$

Table 83: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmaxv23			23.500	$\mathrm{mmol} \cdot \mathrm{l}^{-1} \cdot (3600\ \mathrm{s})^{-1}$	☑
Keqv23			1.050	dimensionless	☑
K1v23			0.418	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
K2v23			0.306	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
K6v23			0.008	dimensionless	☑
K3v23			12.432	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
K5v23			0.411	dimensionless	☑
K4v23			0.005	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
K7v23			48.800	dimensionless	☑

5.25 Reaction vTrAld

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

Name Transaldolase

Reaction equation

$$\mathrm{GraP} + \mathrm{Sed7P} \rightleftharpoons \mathrm{E4P} + \mathrm{Fru6P} \quad (49)$$

Reactants

Table 84: Properties of each reactant.

Id	Name	SBO
GraP	Glyceraldehyde 3-phosphate	
Sed7P	Sedoheptulose 7-phosphate	

Products

Table 85: Properties of each product.

Id	Name	SBO
E4P	Erythrose 4-phosphate	
Fru6P	Fructose 6-phosphate	

Kinetic Law

Derived unit $0.0010000000000000013\ \mathrm{mol} \cdot (3600\ \mathrm{s})^{-1}$

$$v_{25} = \mathrm{vol}\,(\mathrm{compartment}) \cdot \frac{\mathrm{Vmaxv24} \cdot \left([\mathrm{Sed7P}] \cdot [\mathrm{GraP}] - \frac{[\mathrm{E4P}] \cdot [\mathrm{Fru6P}]}{\mathrm{Keqv24}}\right)}{(\mathrm{K1v24} + [\mathrm{GraP}]) \cdot [\mathrm{Sed7P}] + (\mathrm{K2v24} + \mathrm{K6v24} \cdot [\mathrm{Fru6P}]) \cdot [\mathrm{GraP}] + (\mathrm{K3v24} + \mathrm{K5v24} \cdot [\mathrm{Fru6P}]) \cdot [\mathrm{E4P}] + \mathrm{K4v}} \tag{50}$$

Table 86: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmaxv24			27.200	$\mathrm{mmol} \cdot \mathrm{l}^{-1} \cdot (3600\ \mathrm{s})^{-1}$	☑
Keqv24			1.050	dimensionless	☑
K1v24			0.008	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
K2v24			0.048	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
K6v24			0.465	dimensionless	☑
K3v24			0.173	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
K5v24			0.868	dimensionless	☑
K4v24			0.006	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
K7v24			2.524	dimensionless	☑

5.26 Reaction vPPRPPS

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

Name Phosphoribosylpyrophosphate synthetase

Reaction equation

$$\mathrm{MgATP} + \mathrm{Rib5P} \rightleftharpoons \mathrm{MgAMP} + \mathrm{PRPP} \tag{51}$$

Reactants

Table 87: Properties of each reactant.

Id	Name	SBO
MgATP	MgATP	
Rib5P	Ribose 5-phosphate	

Products

Table 88: Properties of each product.

Id	Name	SBO
MgAMP	MgAMP	
PRPP	PRPP	

Kinetic Law

Derived unit $0.0010000000000000013\ \mathrm{mol} \cdot (3600\ \mathrm{s})^{-1}$

$$v_{26} = \mathrm{vol}\,(\mathrm{compartment}) \cdot \frac{\mathrm{Vmaxv25} \cdot \left([\mathrm{Rib5P}] \cdot [\mathrm{MgATP}] - \frac{[\mathrm{PRPP}] \cdot [\mathrm{MgAMP}]}{\mathrm{Keqv25}}\right)}{(\mathrm{KATPv25} + [\mathrm{MgATP}]) \cdot (\mathrm{KR5Pv25} + [\mathrm{Rib5P}])} \tag{52}$$

Table 89: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmaxv25			1.10	$\mathrm{mmol} \cdot \mathrm{l}^{-1} \cdot (3600\ \mathrm{s})^{-1}$	☑
Keqv25			100000.00	dimensionless	☑
KATPv25			0.03	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
KR5Pv25			0.57	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑

5.27 Reaction vTrKet2

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

Name Transketolase 2

Reaction equation

$$\mathrm{Xul5P} + \mathrm{E4P} \rightleftharpoons \mathrm{GraP} + \mathrm{Fru6P} \tag{53}$$

Reactants

Table 90: Properties of each reactant.

Id	Name	SBO
Xul5P	Xylulose 5-phosphate	
E4P	Erythrose 4-phosphate	

Products

Table 91: Properties of each product.

Id	Name	SBO
GraP	Glyceraldehyde 3-phosphate	
Fru6P	Fructose 6-phosphate	

Kinetic Law

Derived unit $0.0010000000000000013\ \mathrm{mol} \cdot (3600\ \mathrm{s})^{-1}$

$$v_{27} = \mathrm{vol}(\mathrm{compartment}) \cdot \frac{\mathrm{Vmaxv26} \cdot \left([\mathrm{E4P}] \cdot [\mathrm{Xul5P}] - \frac{[\mathrm{GraP}] \cdot [\mathrm{Fru6P}]}{\mathrm{Keqv26}}\right)}{(\mathrm{K1v26} + [\mathrm{E4P}]) \cdot [\mathrm{Xul5P}] + (\mathrm{K2v26} + \mathrm{K6v26} \cdot [\mathrm{Fru6P}]) \cdot [\mathrm{E4P}] + (\mathrm{K3v26} + \mathrm{K5v26} \cdot [\mathrm{Fru6P}]) \cdot [\mathrm{GraP}] + \mathrm{K4v} \ldots} \tag{54}$$

Table 92: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmaxv26			23.500	$\mathrm{mmol} \cdot \mathrm{l}^{-1} \cdot (3600\ \mathrm{s})^{-1}$	☑
Keqv26			1.200	dimensionless	☑
K1v26			0.002	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
K2v26			0.306	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
K6v26			0.122	dimensionless	☑
K3v26			0.055	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
K5v26			0.029	dimensionless	☑
K4v26			$3 \cdot 10^{-4}$	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑
K7v26			0.215	dimensionless	☑

5.28 Reaction vPhiexch

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

Name Phosphate exchange

Reaction equation

$$\text{Phiex} \rightleftharpoons \text{Phi} \tag{55}$$

Reactant

Table 93: Properties of each reactant.

Id	Name	SBO
Phiex	Phosphate external	

Product

Table 94: Properties of each product.

Id	Name	SBO
Phi	Phosphate	

Kinetic Law

Derived unit $(3600\ \text{s})^{-1} \cdot \text{mmol}$

$$v_{28} = \text{vol}\,(\text{compartment}) \cdot \text{Vmaxv27} \cdot \left([\text{Phiex}] - \frac{[\text{Phi}]}{\text{Keqv27}} \right) \tag{56}$$

Table 95: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmaxv27			100.0	$(3600\ \text{s})^{-1}$	☑
Keqv27			1.0	dimensionless	☑

5.29 Reaction vLacexch

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

Name Lactate exchange

Reaction equation

$$\text{Lacex} \rightleftharpoons \text{Lac} \tag{57}$$

Reactant

Table 96: Properties of each reactant.

Id	Name	SBO
Lacex	External Lactate	

Product

Table 97: Properties of each product.

Id	Name	SBO
Lac	Lactate	

Kinetic Law

Derived unit $(3600\ \text{s})^{-1} \cdot \text{mmol}$

$$v_{29} = \text{vol}\,(\text{compartment}) \cdot \text{Vmaxv28} \cdot \left([\text{Lacex}] - \frac{[\text{Lac}]}{\text{Keqv28}} \right) \tag{58}$$

Table 98: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmaxv28			10000.0	$(3600\ \text{s})^{-1}$	☑
Keqv28			1.0	dimensionless	☑

5.30 Reaction vPyrexch

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

Name Pyruvate exchange

Reaction equation

$$\text{Pyrex} \rightleftharpoons \text{Pyr} \tag{59}$$

Reactant

Table 99: Properties of each reactant.

Id	Name	SBO
Pyrex	External Pyruvate	

Product

Table 100: Properties of each product.

Id	Name	SBO
Pyr	Pyruvate	

Kinetic Law

Derived unit $(3600\ \mathrm{s})^{-1} \cdot \mathrm{mmol}$

$$v_{30} = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{Vmaxv29} \cdot \left([\mathrm{Pyrex}] - \frac{[\mathrm{Pyr}]}{\mathrm{Keqv29}} \right) \tag{60}$$

Table 101: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmaxv29			10000.0	$(3600\ \mathrm{s})^{-1}$	☑
Keqv29			1.0	dimensionless	☑

5.31 Reaction vMgATP

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

Name MgATP dissociation

Reaction equation

$$\mathrm{MgATP} \rightleftharpoons \mathrm{Mgf} + \mathrm{ATPf} \tag{61}$$

Reactant

Table 102: Properties of each reactant.

Id	Name	SBO
MgATP	MgATP	

Products

Table 103: Properties of each product.

Id	Name	SBO
Mgf	Mg	
ATPf	ATP	

Kinetic Law

Derived unit $(3600\ \mathrm{s})^{-1} \cdot \mathrm{mmol}$

$$v_{31} = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{EqMult} \cdot \left([\mathrm{MgATP}] - \frac{[\mathrm{Mgf}] \cdot [\mathrm{ATPf}]}{\mathrm{KdATP}} \right) \tag{62}$$

Table 104: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
EqMult			10^7	$(3600\ \mathrm{s})^{-1}$	☑
KdATP			0.072	$\mathrm{mmol} \cdot 1^{-1}$	☑

5.32 Reaction vMgADP

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

Name MgADP dissociation

Reaction equation

$$\mathrm{MgADP} \rightleftharpoons \mathrm{Mgf} + \mathrm{ADPf} \tag{63}$$

Reactant

Table 105: Properties of each reactant.

Id	Name	SBO
MgADP	MgADP	

Products

Table 106: Properties of each product.

Id	Name	SBO
Mgf	Mg	
ADPf	ADP	

Kinetic Law

Derived unit $(3600\ \mathrm{s})^{-1} \cdot \mathrm{mmol}$

$$v_{32} = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{EqMult} \cdot \left([\mathrm{MgADP}] - \frac{[\mathrm{Mgf}] \cdot [\mathrm{ADPf}]}{\mathrm{KdADP}} \right) \tag{64}$$

Table 107: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
EqMult			10^7	$(3600\ \mathrm{s})^{-1}$	☑
KdADP			0.760	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑

5.33 Reaction vMgAMP

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

Name MgAMP dissociation

Reaction equation

$$\mathrm{MgAMP} \rightleftharpoons \mathrm{Mgf} + \mathrm{AMPf} \tag{65}$$

Reactant

Table 108: Properties of each reactant.

Id	Name	SBO
MgAMP	MgAMP	

Products

Table 109: Properties of each product.

Id	Name	SBO
Mgf	Mg	
AMPf	AMP	

Kinetic Law

Derived unit $(3600\ \mathrm{s})^{-1} \cdot \mathrm{mmol}$

$$v_{33} = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{EqMult} \cdot \left([\mathrm{MgAMP}] - \frac{[\mathrm{Mgf}] \cdot [\mathrm{AMPf}]}{\mathrm{KdAMP}} \right) \tag{66}$$

Table 110: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
EqMult			10^7	$(3600\ \mathrm{s})^{-1}$	☑
KdAMP			16.640	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑

5.34 Reaction vMgGri23P2

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

Name MgGri23P2 dissociation

Reaction equation

$$\mathrm{MgGri23P2} \rightleftharpoons \mathrm{Mgf} + \mathrm{Gri23P2f} \tag{67}$$

Reactant

Table 111: Properties of each reactant.

Id	Name	SBO
MgGri23P2	MgGri23P2	

Products

Table 112: Properties of each product.

Id	Name	SBO
Mgf	Mg	
Gri23P2f	2,3-Bisphospho-D-glycerate	

Kinetic Law

Derived unit $(3600\ \mathrm{s})^{-1} \cdot \mathrm{mmol}$

$$v_{34} = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{EqMult} \cdot \left([\mathrm{MgGri23P2}] - \frac{[\mathrm{Mgf}] \cdot [\mathrm{Gri23P2f}]}{\mathrm{Kd23P2G}} \right) \tag{68}$$

Table 113: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
EqMult			10^7	$(3600\ \mathrm{s})^{-1}$	☑
Kd23P2G			1.667	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑

5.35 Reaction vP1NADP

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

Name P1NADP dissociation

Reaction equation

$$\mathrm{P1NADP} \rightleftharpoons \mathrm{P1f} + \mathrm{NADPf} \tag{69}$$

Reactant

Table 114: Properties of each reactant.

Id	Name	SBO
P1NADP	Protein1 bound NADP	

Products

Table 115: Properties of each product.

Id	Name	SBO
P1f	Protein1	
NADPf	NADP	

Kinetic Law

Derived unit $(3600\ \mathrm{s})^{-1} \cdot \mathrm{mmol}$

$$v_{35} = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{EqMult} \cdot \left([\mathrm{P1NADP}] - \frac{[\mathrm{P1f}] \cdot [\mathrm{NADPf}]}{\mathrm{Kd1}} \right) \tag{70}$$

Table 116: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
EqMult			10^{7}	$(3600\ \mathrm{s})^{-1}$	☑
Kd1			$2 \cdot 10^{-4}$	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑

5.36 Reaction vP1NADPH

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

Name P1NADPH dissociation

Reaction equation

$$\mathrm{P1NADPH} \rightleftharpoons \mathrm{P1f} + \mathrm{NADPHf} \tag{71}$$

Reactant

Table 117: Properties of each reactant.

Id	Name	SBO
P1NADPH	Protein1 bound NADPH	

Products

Table 118: Properties of each product.

Id	Name	SBO
P1f	Protein1	
NADPHf	NADPH	

Kinetic Law

Derived unit $(3600\ \mathrm{s})^{-1} \cdot \mathrm{mmol}$

$$v_{36} = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{EqMult} \cdot \left([\mathrm{P1NADPH}] - \frac{[\mathrm{P1f}] \cdot [\mathrm{NADPHf}]}{\mathrm{Kd3}} \right) \tag{72}$$

Table 119: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
EqMult			10^{7}	$(3600\ \mathrm{s})^{-1}$	☑
Kd3			10^{-5}	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑

5.37 Reaction vP2NADP

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

Name P2NADP dissociation

Reaction equation

$$\mathrm{P2NADP} \rightleftharpoons \mathrm{P2f} + \mathrm{NADPf} \tag{73}$$

Reactant

Table 120: Properties of each reactant.

Id	Name	SBO
P2NADP	Protein2 bound NADP	

Products

Table 121: Properties of each product.

Id	Name	SBO
P2f	Protein2	
NADPf	NADP	

Kinetic Law

Derived unit $(3600\ \mathrm{s})^{-1} \cdot \mathrm{mmol}$

$$v_{37} = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{EqMult} \cdot \left([\mathrm{P2NADP}] - \frac{[\mathrm{P2f}] \cdot [\mathrm{NADPf}]}{\mathrm{Kd2}} \right) \tag{74}$$

Table 122: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
EqMult			10^{7}	$(3600\ \mathrm{s})^{-1}$	☑
Kd2			10^{-5}	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑

5.38 Reaction vP2NADPH

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

Name P2NADPH dissociation

Reaction equation

$$\mathrm{P2NADPH} \rightleftharpoons \mathrm{P2f} + \mathrm{NADPHf} \tag{75}$$

Reactant

Table 123: Properties of each reactant.

Id	Name	SBO
P2NADPH	Protein2 bound NADPH	

Products

Table 124: Properties of each product.

Id	Name	SBO
P2f	Protein2	
NADPHf	NADPH	

Kinetic Law

Derived unit $(3600\ \mathrm{s})^{-1} \cdot \mathrm{mmol}$

$$v_{38} = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{EqMult} \cdot \left([\mathrm{P2NADPH}] - \frac{[\mathrm{P2f}] \cdot [\mathrm{NADPHf}]}{\mathrm{Kd4}} \right) \tag{76}$$

Table 125: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
EqMult			10^{7}	$(3600\ \mathrm{s})^{-1}$	☑
Kd4			$2 \cdot 10^{-4}$	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑

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 Glcin

Name Glucose in

Initial concentration $4.5663\ \mathrm{mmol} \cdot \mathrm{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Glcin} = v_1 - v_2 \tag{77}$$

6.2 Species MgATP

Name MgATP

Initial concentration $1.4\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in ten reactions (as a reactant in vHEX, vPFK, vATPase, vAK, vPPRPPS, vMgATP and as a product in vPGK, vPK and as a modifier in vG6PDH, vPGLDH).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{MgATP} = v_8 + v_{13} - v_2 - v_4 - v_{16} - v_{17} - v_{26} - v_{31} \tag{78}$$

6.3 Species Glc6P

Name Glucose 6-phosphate

Initial concentration $0.0394\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Glc6P} = v_2 - v_3 - v_{18} \tag{79}$$

6.4 Species MgADP

Name MgADP

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

This species takes part in seven reactions (as a reactant in vPGK, vPK, vMgADP and as a product in vHEX, vPFK, vATPase, vAK).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{MgADP} = v_2 + v_4 + v_{16} + v_{17} - v_8 - v_{13} - v_{32} \tag{80}$$

6.5 Species Fru6P

Name Fructose 6-phosphate

Initial concentration $0.0153\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in four reactions (as a reactant in vPFK and as a product in vGPI, vTrAld, vTrKet2).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Fru6P} = v_3 + v_{25} + v_{27} - v_4 \tag{81}$$

6.6 Species Fru16P2

Name Fructose 1,6-phosphate

Initial concentration $0.0097\ \text{mmol} \cdot \text{l}^{-1}$

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

$$\frac{\text{d}}{\text{d}t}\text{Fru16P2} = v_4 - v_5 \tag{82}$$

6.7 Species GraP

Name Glyceraldehyde 3-phosphate

Initial concentration $0.0061\ \text{mmol} \cdot \text{l}^{-1}$

This species takes part in six reactions (as a reactant in vGAPDH, vTrAld and as a product in vALD, vTPI, vTrKet1, vTrKet2).

$$\frac{\text{d}}{\text{d}t}\text{GraP} = v_5 + v_6 + v_{24} + v_{27} - v_7 - v_{25} \tag{83}$$

6.8 Species DHAP

Name Dihydroxyacetone phosphate

Initial concentration $0.1492\ \text{mmol} \cdot \text{l}^{-1}$

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

$$\frac{\text{d}}{\text{d}t}\text{DHAP} = v_5 - v_6 \tag{84}$$

6.9 Species Phi

Name Phosphate

Initial concentration $0.9992\ \text{mmol} \cdot \text{l}^{-1}$

This species takes part in four reactions (as a reactant in vGAPDH and as a product in vBPGP, vATPase, vPhiexch).

$$\frac{\text{d}}{\text{d}t}\text{Phi} = v_{10} + v_{16} + v_{28} - v_7 \tag{85}$$

6.10 Species NAD

Name NAD

Initial concentration $0.0653\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{NAD} = v_{14} - v_7 \tag{86}$$

6.11 Species Gri13P2

Name 1,3-Bisphospho-D-glycerate

Initial concentration $5\cdot 10^{-4}\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Gri13P2} = v_7 - v_8 - v_9 \tag{87}$$

6.12 Species NADH

Name NADH

Initial concentration $2\cdot 10^{-4}\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{NADH} = v_7 - v_{14} \tag{88}$$

6.13 Species Gri3P

Name 3-Phospho-D-glycerate

Initial concentration $0.0658\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Gri3P} = v_8 + v_{10} - v_{11} \tag{89}$$

6.14 Species Gri23P2f

Name 2,3-Bisphospho-D-glycerate

Initial concentration $2.0601\ \text{mmol} \cdot \text{l}^{-1}$

This species takes part in six reactions (as a reactant in vBPGP and as a product in vBPGM, vMgGri23P2 and as a modifier in vHEX, vG6PDH, vPGLDH).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Gri23P2f} = v_9 + v_{34} - v_{10} \tag{90}$$

6.15 Species Gri2P

Name 2-Phospho-D-glycerate

Initial concentration $0.0084\ \text{mmol} \cdot \text{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Gri2P} = v_{11} - v_{12} \tag{91}$$

6.16 Species PEP

Name Phosphoenolpyruvate

Initial concentration $0.0109\ \text{mmol} \cdot \text{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{PEP} = v_{12} - v_{13} \tag{92}$$

6.17 Species Pyr

Name Pyruvate

Initial concentration $0.084\ \text{mmol} \cdot \text{l}^{-1}$

This species takes part in four reactions (as a reactant in vLDHNADH, vLDHNADPH and as a product in vPK, vPyrexch).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Pyr} = v_{13} + v_{30} - v_{14} - v_{15} \tag{93}$$

6.18 Species Lac

Name Lactate

Initial concentration $1.6803\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in three reactions (as a product in vLDHNADH, vLDHNADPH, vLacexch).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Lac} = v_{14} + v_{15} + v_{29} \tag{94}$$

6.19 Species NADPHf

Name NADPH

Initial concentration $0.0040\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in six reactions (as a reactant in vLDHNADPH, vGSSGRD and as a product in vG6PDH, vPGLDH, vP1NADPH, vP2NADPH).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{NADPHf} = v_{18} + v_{19} + v_{36} + v_{38} - v_{15} - v_{20} \tag{95}$$

6.20 Species NADPf

Name NADP

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

This species takes part in six reactions (as a reactant in vG6PDH, vPGLDH and as a product in vLDHNADPH, vGSSGRD, vP1NADP, vP2NADP).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{NADPf} = v_{15} + v_{20} + v_{35} + v_{37} - v_{18} - v_{19} \tag{96}$$

6.21 Species AMPf

Name AMP

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{AMPf} = v_{33} - v_{17} \tag{97}$$

6.22 Species ADPf

Name ADP

Initial concentration $0.25\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a product in vAK, vMgADP).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ADPf} = v_{17} + v_{32} \tag{98}$$

6.23 Species GlcA6P

Name Phospho-D-glucono-1,5-lactone

Initial concentration $0.025\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{GlcA6P} = v_{18} - v_{19} \tag{99}$$

6.24 Species Rul5P

Name Ribulose 5-phosphate

Initial concentration $0.0047\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in three reactions (as a reactant in vRibPepi, vRibPiso and as a product in vPGLDH).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Rul5P} = v_{19} - v_{22} - v_{23} \tag{100}$$

6.25 Species GSSG

Name Oxidized Glutathione

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

This species takes part in two reactions (as a reactant in vGSSGRD and as a product in vGSHox).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{GSSG} = v_{21} - v_{20} \tag{101}$$

6.26 Species GSH

Name Reduced Glutathione

Initial concentration $3.1136\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in vGSHox and as a product in vGSSGRD).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{GSH} = 2v_{20} - 2v_{21} \tag{102}$$

6.27 Species Xul5P

Name Xylulose 5-phosphate

Initial concentration $0.0127\ \text{mmol} \cdot \text{l}^{-1}$

This species takes part in three reactions (as a reactant in vTrKet1, vTrKet2 and as a product in vRibPepi).

$$\frac{\text{d}}{\text{d}t}\text{Xul5P} = v_{22} - v_{24} - v_{27} \tag{103}$$

6.28 Species Rib5P

Name Ribose 5-phosphate

Initial concentration $0.014\ \text{mmol} \cdot \text{l}^{-1}$

This species takes part in three reactions (as a reactant in vTrKet1, vPPRPPS and as a product in vRibPiso).

$$\frac{\text{d}}{\text{d}t}\text{Rib5P} = v_{23} - v_{24} - v_{26} \tag{104}$$

6.29 Species Sed7P

Name Sedoheptulose 7-phosphate

Initial concentration $0.0154\ \text{mmol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a reactant in vTrAld and as a product in vTrKet1).

$$\frac{\text{d}}{\text{d}t}\text{Sed7P} = v_{24} - v_{25} \tag{105}$$

6.30 Species E4P

Name Erythrose 4-phosphate

Initial concentration $0.0063\ \text{mmol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a reactant in vTrKet2 and as a product in vTrAld).

$$\frac{\text{d}}{\text{d}t}\text{E4P} = v_{25} - v_{27} \tag{106}$$

6.31 Species MgAMP

Name MgAMP

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

This species takes part in three reactions (as a reactant in vMgAMP and as a product in vPPRPPS and as a modifier in vPFK).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{MgAMP} = v_{26} - v_{33} \tag{107}$$

6.32 Species ATPf

Name ATP

Initial concentration $0.25\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in five reactions (as a product in vMgATP and as a modifier in vPFK, vPK, vG6PDH, vPGLDH).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ATPf} = v_{31} \tag{108}$$

6.33 Species Mgf

Name Mg

Initial concentration $0.8\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in six reactions (as a product in vMgATP, vMgADP, vMgAMP, vMgGri23P2 and as a modifier in vHEX, vPFK).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Mgf} = v_{31} + v_{32} + v_{33} + v_{34} \tag{109}$$

6.34 Species MgGri23P2

Name MgGri23P2

Initial concentration $0.5\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in six reactions (as a reactant in vMgGri23P2 and as a modifier in vHEX, vBPGM, vBPGP, vG6PDH, vPGLDH).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{MgGri23P2} = -v_{34} \tag{110}$$

6.35 Species P1NADP

Name Protein1 bound NADP

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

This species takes part in one reaction (as a reactant in vP1NADP).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{P1NADP} = -v_{35} \tag{111}$$

6.36 Species P1f

Name Protein1

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

This species takes part in two reactions (as a product in vP1NADP, vP1NADPH).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{P1f} = v_{35} + v_{36} \tag{112}$$

6.37 Species P1NADPH

Name Protein1 bound NADPH

Initial concentration $0.024\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in one reaction (as a reactant in vP1NADPH).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{P1NADPH} = -v_{36} \tag{113}$$

6.38 Species P2NADP

Name Protein2 bound NADP

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

This species takes part in one reaction (as a reactant in vP2NADP).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{P2NADP} = -v_{37} \tag{114}$$

6.39 Species P2f

Name Protein2

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

This species takes part in two reactions (as a product in vP2NADP, vP2NADPH).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{P2f} = v_{37} + v_{38} \tag{115}$$

6.40 Species P2NADPH

Name Protein2 bound NADPH

Initial concentration $0.024\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in one reaction (as a reactant in vP2NADPH).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{P2NADPH} = -v_{38} \tag{116}$$

6.41 Species PRPP

Name PRPP

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{PRPP} = 0 \tag{117}$$

6.42 Species Lacex

Name External Lactate

Initial concentration $1.68\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Lacex} = 0 \tag{118}$$

6.43 Species Pyrex

Name External Pyruvate

Initial concentration $0.084\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Pyrex} = 0 \tag{119}$$

6.44 Species Glcout

Name Glucose outside

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

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:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Glcout} = 0 \tag{120}$$

6.45 Species Phiex

Name Phosphate external

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Phiex} = 0 \tag{121}$$

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