

SBML Model Report

Model name: “Kerkhoven2013 - Glycolysis in T.brucei - MODEL A”



May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by the following two authors: Vijayalakshmi Chelliah¹ and Eduard Kerkhoven² at February tenth 2014 at 10:29 a. m. and last time modified at March fifth 2014 at 3:57 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	3
species types	0	species	31
events	0	constraints	0
reactions	21	function definitions	7
global parameters	0	unit definitions	5
rules	0	initial assignments	0

Model Notes

Kerkhoven2013 - Glycolysis in T.brucei - MODEL A

There are six models (Model A, B, C, C-fruc, D, D-fruc) described in the paper. Model A ([BIOMD0000000513](#)) is the model developed originally by Achar et al. (2012) ([BIOMD0000000428](#)), which describes glycolysis in T.brucei. This glycolysis model is extended to include pentose

¹EMBL-EBI, viji@ebi.ac.uk

²Chalmers University of Technology, eduardk@chalmers.se

phosphate pathway (PPP), which is Model B (([BIOMD0000000514](#)). Model B is further extended to include glycosomal ribokinase, leading to Model C ([BIOMD0000000510](#)). Model D ([BIOMD0000000511](#)) is again an extension of Model B, which includes an ATP:ADP antiporter. Model C-fruc ([BIOMD0000000515](#)) and Model D-fruc ([BIOMD0000000516](#)) are extensions of Model C and D, respectively, which includes fructose transporter and its subsequent utilizing reactions. This model correspond to Model A of the paper.

This model is described in the article:[Handling uncertainty in dynamic models: the pentose phosphate pathway in Trypanosoma brucei](#).Kerkhoven EJ, Achcar F, Alibu VP, Burchmore RJ, Gilbert IH, Trybio M, Driessen NN, Gilbert D, Breitling R, Bakker BM, Barrett MP.PLoS Comput Biol. 2013 Dec;9(12):e1003371.

Abstract:

Dynamic models of metabolism can be useful in identifying potential drug targets, especially in unicellular organisms. A model of glycolysis in the causative agent of human African trypanosomiasis, *Trypanosoma brucei*, has already shown the utility of this approach. Here we add the pentose phosphate pathway (PPP) of *T. brucei* to the glycolytic model. The PPP is localized to both the cytosol and the glycosome and adding it to the glycolytic model without further adjustments leads to a draining of the essential bound-phosphate moiety within the glycosome. This phosphate „leak,, must be resolved for the model to be a reasonable representation of parasite physiology. Two main types of theoretical solution to the problem could be identified: (i) including additional enzymatic reactions in the glycosome, or (ii) adding a mechanism to transfer bound phosphates between cytosol and glycosome. One example of the first type of solution would be the presence of a glycosomal ribokinase to regenerate ATP from ribose 5-phosphate and ADP. Experimental characterization of ribokinase in *T. brucei* showed that very low enzyme levels are sufficient for parasite survival, indicating that other mechanisms are required in controlling the phosphate leak. Examples of the second type would involve the presence of an ATP:ADP exchanger or recently described permeability pores in the glycosomal membrane, although the current absence of identified genes encoding such molecules impedes experimental testing by genetic manipulation. Confronted with this uncertainty, we present a modeling strategy that identifies robust predictions in the context of incomplete system characterization. We illustrate this strategy by exploring the mechanism underlying the essential function of one of the PPP enzymes, and validate it by confirming the model predictions experimentally.

This model is hosted on [BioModels Database](#) and identifiedby: [BIOMD0000000513](#) .

To cite BioModels Database, please use: [BioModels Database: An enhanced, curated and annotated resourcefor published quantitative kinetic models](#) .

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2 Unit Definitions

This is an overview of five unit definitions.

2.1 Unit volume

Definition μl

2.2 Unit length

Definition m

2.3 Unit substance

Definition nmol

2.4 Unit time

Definition 60 s

2.5 Unit area

Definition m^2

3 Compartments

This model contains three compartments.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
cytosol	cytosol	0000290	3	5.4549	μl	<input checked="" type="checkbox"/>	
glycosome	glycosome	0000290	3	0.2451	μl	<input checked="" type="checkbox"/>	
default	default	0000290	3	1	litre	<input checked="" type="checkbox"/>	

3.1 Compartment cytosol

This is a three dimensional compartment with a constant size of 5.4549 μl .

Name cytosol

SBO:0000290 physical compartment

3.2 Compartment glycosome

This is a three dimensional compartment with a constant size of 0.2451 μl .

Name glycosome

SBO:0000290 physical compartment

3.3 Compartment default

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

Name default

SBO:0000290 physical compartment

4 Species

This model contains 31 species. The boundary condition of seven of these species is set to true so that these species' amount cannot be changed by any reaction. Section 7 provides further details and the derived rates of change of each species.

Table 3: Properties of each species.

Id	Name	Compartment	Derived Unit	Constant	Boundary Condi- tion
_2PGA_c	_2PGA_c	cytosol	$\text{nmol} \cdot \mu\text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
DHAP_c	DHAP_c	cytosol	$\text{nmol} \cdot \mu\text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
ATP_g	ATP_g	glycosome	$\text{nmol} \cdot \mu\text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
DHAP_g	DHAP_g	glycosome	$\text{nmol} \cdot \mu\text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
ADP_g	ADP_g	glycosome	$\text{nmol} \cdot \mu\text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
Glc6P_g	Glc6P_g	glycosome	$\text{nmol} \cdot \mu\text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
ADP_c	ADP_c	cytosol	$\text{nmol} \cdot \mu\text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
_3PGA_c	_3PGA_c	cytosol	$\text{nmol} \cdot \mu\text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
Fru6P_g	Fru6P_g	glycosome	$\text{nmol} \cdot \mu\text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
Pi_g	Pi_g	glycosome	$\text{nmol} \cdot \mu\text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
O2_c	O2_c	default	$\text{nmol} \cdot \mu\text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
Gly_e	Gly_e	default	$\text{nmol} \cdot \mu\text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
ATP_c	ATP_c	cytosol	$\text{nmol} \cdot \mu\text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
_13BPGA_g	_13BPGA_g	glycosome	$\text{nmol} \cdot \mu\text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
Glc_c	Glc_c	cytosol	$\text{nmol} \cdot \mu\text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
Glc_e	Glc_e	default	$\text{nmol} \cdot \mu\text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
Glc_g	Glc_g	glycosome	$\text{nmol} \cdot \mu\text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
Pyr_c	Pyr_c	cytosol	$\text{nmol} \cdot \mu\text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
Pyr_e	Pyr_e	default	$\text{nmol} \cdot \mu\text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
NAD_g	NAD_g	glycosome	$\text{nmol} \cdot \mu\text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
Fru16BP_g	Fru16BP_g	glycosome	$\text{nmol} \cdot \mu\text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>

Id	Name	Compartment	Derived Unit	Constant	Boundary Condition
GA3P_g	GA3P_g	glycosome	$\text{nmol} \cdot \mu\text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
CO2_c	CO2_c	cytosol	$\text{nmol} \cdot \mu\text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
CO2_g	CO2_g	glycosome	$\text{nmol} \cdot \mu\text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
Gly3P_c	Gly3P_c	cytosol	$\text{nmol} \cdot \mu\text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
Gly3P_g	Gly3P_g	glycosome	$\text{nmol} \cdot \mu\text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
PEP_c	PEP_c	cytosol	$\text{nmol} \cdot \mu\text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
AMP_g	AMP_g	glycosome	$\text{nmol} \cdot \mu\text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
_3PGA_g	_3PGA_g	glycosome	$\text{nmol} \cdot \mu\text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
AMP_c	AMP_c	cytosol	$\text{nmol} \cdot \mu\text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
NADH_g	NADH_g	glycosome	$\text{nmol} \cdot \mu\text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>

5 Function definitions

This is an overview of seven function definitions.

5.1 Function definition `vAK`

Name `vAK`

Arguments ADP, AMP, ATP, k1, k2

Mathematical Expression

$$k1 \cdot \text{ADP}^2 - \text{AMP} \cdot \text{ATP} \cdot k2 \quad (1)$$

5.2 Function definition `v2sub2prod`

Name `v2sub2prod`

Arguments V_{fmax}, K_{eq}, S1, K_{s1}, S2, K_{s2}, P1, K_{p1}, P2, K_{p2}

Mathematical Expression

$$\frac{V_{fmax} \cdot S1 \cdot S2 \cdot \left(1 - \frac{P1 \cdot P2}{K_{eq} \cdot S1 \cdot S2}\right)}{K_{s1} \cdot K_{s2} \cdot \left(1 + \frac{S1}{K_{s1}} + \frac{P1}{K_{p1}}\right) \cdot \left(1 + \frac{S2}{K_{s2}} + \frac{P2}{K_{p2}}\right)} \quad (2)$$

5.3 Function definition `v1sub`

Name `v1sub`

Arguments V_{fmax}, S, K_s

Mathematical Expression

$$\frac{V_{fmax} \cdot S}{K_s \cdot \left(1 + \frac{S}{K_s}\right)} \quad (3)$$

5.4 Function definition `v2sub2prod_compinh`

Name `v2sub2prod_compinh`

Arguments V_{fmax}, K_{eq}, S1, K_{s1}, S2, K_{s2}, P1, K_{p1}, P2, K_{p2}, I1, K_{i1}, I2, K_{i2}

Mathematical Expression

$$\frac{V_{fmax} \cdot S1 \cdot S2 \cdot \left(1 - \frac{P1 \cdot P2}{K_{eq} \cdot S1 \cdot S2}\right)}{K_{s1} \cdot K_{s2} \cdot \left(1 + \frac{S1}{K_{s1}} + \frac{P1}{K_{p1}}\right) \cdot \left(1 + \frac{S2}{K_{s2}} + \frac{P2}{K_{p2}} + \frac{I1}{K_{i1}} + \frac{I2}{K_{i2}}\right)} \quad (4)$$

5.5 Function definition `mass_action_rev`

Name `mass_action_rev`

Arguments `k1`, `S`, `k2`, `P`

Mathematical Expression

$$k1 \cdot S - k2 \cdot P \quad (5)$$

5.6 Function definition `v1sub1prod`

Name `v1sub1prod`

Arguments `Vfmax`, `Keq`, `S`, `Ks`, `P`, `Kp`

Mathematical Expression

$$\frac{V_{fmax} \cdot S \cdot \left(1 - \frac{P}{K_{eq} \cdot S}\right)}{K_s \cdot \left(1 + \frac{S}{K_s} + \frac{P}{K_p}\right)} \quad (6)$$

5.7 Function definition `mass_action_irrev`

Name `mass_action_irrev`

Arguments `k`, `S`

Mathematical Expression

$$k \cdot S \quad (7)$$

6 Reactions

This model contains 21 reactions. All reactions are listed in the following table and are subsequently described in detail. If a reaction is affected by a modifier, the identifier of this species is written above the reaction arrow.

Table 4: Overview of all reactions

Nº	Id	Name	Reaction Equation	SBO
1	TPI_g	TPI_g	$\text{DHAP}_g \xrightleftharpoons[\text{GA3P}_g]{\text{DHAP}_g, \text{GA3P}_g, \text{DHAP}_g, \text{GA3P}_g} \text{GA3P}_g$	
2	PYK_c	PYK_c	$\text{PEP}_c + \text{ADP}_c \xrightleftharpoons[\text{ATP}_c]{\text{ADP}_c, \text{Pyr}_c, \text{ATP}_c, \text{PEP}_c, \text{ADP}_c, \text{Pyr}_c, \text{ATP}_c, \text{PEP}_c} \text{Pyr}_c + \text{ATP}_c$	
3	PFK_g	PFK_g	$\text{ATP}_g + \text{Fru6P}_g \xrightleftharpoons[\text{ADP}_g]{\text{Fru6P}_g, \text{ATP}_g, \text{Fru16BP}_g, \text{ADP}_g, \text{Fru6P}_g, \text{ATP}_g, \text{Fru16BP}_g, \text{ADP}_g} \text{ADP}_g$	
4	GlcT_g	GlcT_g	$\text{Glc}_c \xrightleftharpoons[\text{Glc}_g]{\text{Glc}_c, \text{Glc}_g, \text{Glc}_c, \text{Glc}_g} \text{Glc}_g$	
5	PGAM_c	PGAM_c	$\text{_3PGA}_c \xrightleftharpoons[\text{_2PGA}_c]{\text{_3PGA}_c, \text{_2PGA}_c, \text{_3PGA}_c, \text{_2PGA}_c} \text{_2PGA}_c$	
6	PyrT_c	PyrT_c	$\text{Pyr}_c \xrightarrow[\text{Pyr}_e]{\text{Pyr}_c, \text{Pyr}_c} \text{Pyr}_e$	
7	GlcT_c	GlcT_c	$\text{Glc}_e \xrightleftharpoons[\text{Glc}_c]{\text{Glc}_e, \text{Glc}_c, \text{Glc}_e, \text{Glc}_c} \text{Glc}_c$	
8	ALD_g	ALD_g	$\text{Fru16BP}_g \xrightleftharpoons[\text{DHAP}_g]{\text{ATP}_g, \text{ADP}_g, \text{AMP}_g, \text{Fru16BP}_g, \text{GA3P}_g, \text{DHAP}_g, \text{ATP}_g, \text{ADP}_g, \text{AMP}_g} \text{DHAP}_g$	
9	ENO_c	ENO_c	$\text{_2PGA}_c \xrightleftharpoons[\text{PEP}_c]{\text{_2PGA}_c, \text{PEP}_c, \text{_2PGA}_c, \text{PEP}_c} \text{PEP}_c$	
10	H XK_g	H XK_g	$\text{ATP}_g + \text{Glc}_g \xrightleftharpoons[\text{ADP}_g]{\text{Glc}_g, \text{ATP}_g, \text{Glc6P}_g, \text{ADP}_g, \text{Glc}_g, \text{ATP}_g, \text{Glc6P}_g, \text{ADP}_g} \text{Glc6P}_g$	
11	_3PGAT_g	_3PGAT_g	$\text{_3PGA}_g \xrightleftharpoons[\text{_3PGA}_c]{\text{_3PGA}_g, \text{_3PGA}_c, \text{_3PGA}_g, \text{_3PGA}_c} \text{_3PGA}_c$	

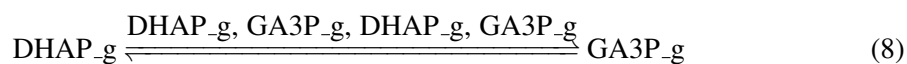
Nº	Id	Name	Reaction Equation	SBO
12	PGK_g	PGK_g	$\text{13BPGA_g} + \text{ADP_g} \xrightleftharpoons{\text{13BPGA_g, ADP_g, 3PGA_g, ATP_g, 13BPGA_g, ADP_g, 3PGA_g, ATP_g}} \text{ATP_g}$	
13	G3PDH_g	G3PDH_g	$\text{NADH_g} + \text{DHAP_g} \xrightleftharpoons{\text{DHAP_g, NADH_g, Gly3P_g, NAD_g, DHAP_g, NADH_g, Gly3P_g, NAD_g}} \text{NAD_g}$	
14	GPO_c	GPO_c	$\text{Gly3P_c} \xrightarrow{\text{Gly3P_c, Gly3P_c}} \text{DHAP_c}$	
15	ATPu_c	ATPu_c	$\text{ATP_c} \xrightarrow{\text{ATP_c, ADP_c, ATP_c, ADP_c}} \text{ADP_c}$	
16	GK_g	GK_g	$\text{Gly3P_g} + \text{ADP_g} \xrightleftharpoons{\text{Gly3P_g, ADP_g, Gly_e, ATP_g, Gly3P_g, ADP_g, Gly_e, ATP_g}} \text{ATP_g}$	
17	AK_c	AK_c	$2 \text{ADP_c} \xrightleftharpoons{\text{ADP_c, AMP_c, ATP_c, ADP_c, AMP_c, ATP_c}} \text{AMP_c} + \text{ATP_c}$	
18	PGI_g	PGI_g	$\text{Glc6P_g} \xrightleftharpoons{\text{Glc6P_g, Fru6P_g, Glc6P_g, Fru6P_g}} \text{Fru6P_g}$	
19	GAPDH_g	GAPDH_g	$\text{GA3P_g} + \text{NAD_g} \xrightleftharpoons{\text{GA3P_g, NAD_g, 13BPGA_g, NADH_g, GA3P_g, NAD_g, 13BPGA_g, NADH_g}} \text{Pi_g}$	
20	AK_g	AK_g	$2 \text{ADP_g} \xrightleftharpoons{\text{ADP_g, AMP_g, ATP_g, ADP_g, AMP_g, ATP_g}} \text{AMP_g} + \text{ATP_g}$	
21	GDA_g	GDA_g	$\text{Gly3P_g} + \text{DHAP_c} \xrightleftharpoons{\text{Gly3P_g, DHAP_c, Gly3P_c, DHAP_g, Gly3P_g, DHAP_c, Gly3P_c, DHAP_g}} \text{DHAP_g}$	

6.1 Reaction TPI_g

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

Name TPI_g

Reaction equation



Reactant

Table 5: Properties of each reactant.

Id	Name	SBO
DHAP_g	DHAP_g	

Modifiers

Table 6: Properties of each modifier.

Id	Name	SBO
DHAP_g	DHAP_g	
GA3P_g	GA3P_g	
DHAP_g	DHAP_g	
GA3P_g	GA3P_g	

Product

Table 7: Properties of each product.

Id	Name	SBO
GA3P_g	GA3P_g	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = v_{1\text{sub1prod}}(\text{TPI_g_Vmax}, \text{TPI_g_Keq}, [\text{DHAP_g}], \text{TPI_g_KmDHAP}, [\text{GA3P_g}], \text{TPI_g_KmGA3P}) \quad (9)$$

$$v_{\text{sub1prod}}(V_{\text{fmax}}, K_{\text{eq}}, S, K_{\text{s}}, P, K_{\text{p}}) = \frac{V_{\text{fmax}} \cdot S \cdot \left(1 - \frac{P}{K_{\text{eq}} \cdot S}\right)}{K_{\text{s}} \cdot \left(1 + \frac{S}{K_{\text{s}}} + \frac{P}{K_{\text{p}}}\right)} \quad (10)$$

Table 8: Properties of each parameter.

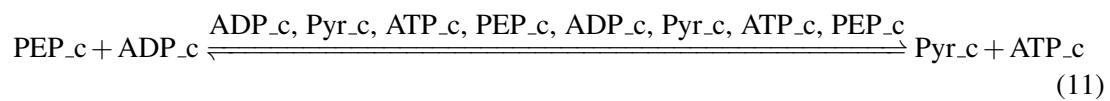
Id	Name	SBO	Value	Unit	Constant
TPI_g_Vmax	TPI_g_Vmax		999.300		✓
TPI_g_Keq	TPI_g_Keq		0.046		✓
TPI_g_KmDHAP	TPI_g_KmDHAP		1.200		✓
TPI_g_KmGA3P	TPI_g_KmGA3P		0.250		✓

6.2 Reaction PYK_c

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

Name PYK_c

Reaction equation



Reactants

Table 9: Properties of each reactant.

Id	Name	SBO
PEP_c	PEP_c	
ADP_c	ADP_c	

Modifiers

Table 10: Properties of each modifier.

Id	Name	SBO
ADP_c	ADP_c	
Pyr_c	Pyr_c	
ATP_c	ATP_c	
PEP_c	PEP_c	
ADP_c	ADP_c	

Id	Name	SBO
Pyr_c	Pyr_c	
ATP_c	ATP_c	
PEP_c	PEP_c	

Products

Table 11: Properties of each product.

Id	Name	SBO
Pyr_c	Pyr_c	
ATP_c	ATP_c	

Kinetic Law

Derived unit contains undeclared units

$$\begin{aligned}
 v_2 &= \frac{\text{PYK_c_Vmax} \cdot [\text{ADP_c}] \cdot \left(1 - \frac{[\text{Pyr_c}] \cdot [\text{ATP_c}]}{\text{PYK_c_Keq} \cdot [\text{PEP_c}] \cdot [\text{ADP_c}]}\right) \cdot \left(\frac{[\text{PEP_c}]}{\text{PYK_c_KmPEP} \cdot \left(1 + \frac{[\text{ADP_c}]}{\text{PYK_c_KiADP}} + \frac{[\text{ATP_c}]}{\text{PYK_c_KiATP}}\right)}\right)^{\text{PYK_c_n}}}{\text{PYK_c_KmADP} \cdot \left(1 + \left(\frac{[\text{PEP_c}]}{\text{PYK_c_KmPEP} \cdot \left(1 + \frac{[\text{ADP_c}]}{\text{PYK_c_KiADP}} + \frac{[\text{ATP_c}]}{\text{PYK_c_KiATP}}\right)}\right)^{\text{PYK_c_n}} + \frac{[\text{Pyr_c}]}{\text{PYK_c_KmPyr}}\right) \cdot \left(1 + \frac{[\text{ADP_c}]}{\text{PYK_c_KmADP}} + \frac{[\text{ATP_c}]}{\text{PYK_c_KmATP}}\right)} \quad (12)
 \end{aligned}$$

Table 12: Properties of each parameter.

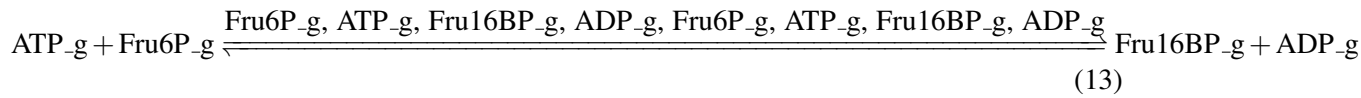
Id	Name	SBO	Value	Unit	Constant
PYK_c_Vmax	PYK_c_Vmax		1020.000		✓
PYK_c_KmPEP	PYK_c_KmPEP		0.340		✓
PYK_c_KiATP	PYK_c_KiATP		0.570		✓
PYK_c_KiADP	PYK_c_KiADP		0.640		✓
PYK_c_n	PYK_c_n		2.500		✓
PYK_c_KmADP	PYK_c_KmADP		0.114		✓
PYK_c_Keq	PYK_c_Keq		10800.000		✓
PYK_c_KmPyr	PYK_c_KmPyr		50.000		✓
PYK_c_KmATP	PYK_c_KmATP		15.000		✓

6.3 Reaction PFK_g

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

Name PFK_g

Reaction equation



Reactants

Table 13: Properties of each reactant.

Id	Name	SBO
ATP _g	ATP _g	
Fru6P _g	Fru6P _g	

Modifiers

Table 14: Properties of each modifier.

Id	Name	SBO
Fru6P _g	Fru6P _g	
ATP _g	ATP _g	
Fru16BP _g	Fru16BP _g	
ADP _g	ADP _g	
Fru6P _g	Fru6P _g	
ATP _g	ATP _g	
Fru16BP _g	Fru16BP _g	
ADP _g	ADP _g	

Products

Table 15: Properties of each product.

Id	Name	SBO
Fru16BP _g	Fru16BP _g	
ADP _g	ADP _g	

Kinetic Law

Derived unit contains undeclared units

v_3

(14)

$$= \frac{\text{PFK_g_Vmax} \cdot \text{PFK_g_Ki1} \cdot [\text{Fru6P_g}] \cdot [\text{ATP_g}] \cdot \left(1 - \frac{[\text{Fru6P_g}]}{\text{PFK_g_Vmax}}\right)}{\text{PFK_g_KmFru6P} \cdot \text{PFK_g_KmATP} \cdot ([\text{Fru6BP_g}] + \text{PFK_g_Ki1}) \cdot \left(\frac{\text{PFK_g_KsATP}}{\text{PFK_g_KmATP}} + \frac{[\text{Fru6P_g}]}{\text{PFK_g_KmFru6P}} + \frac{[\text{ATP_g}]}{\text{PFK_g_KmATP}}\right)}$$

Table 16: Properties of each parameter.

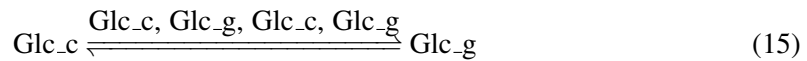
Id	Name	SBO	Value	Unit	Constant
PFK_g_Vmax	PFK_g_Vmax		1708.000		✓
PFK_g_Ki1	PFK_g_Ki1		15.800		✓
PFK_g_KmFru6P	PFK_g_KmFru6P		0.999		✓
PFK_g_KmATP	PFK_g_KmATP		0.065		✓
PFK_g_Keq	PFK_g_Keq		1035.000		✓
PFK_g_KsATP	PFK_g_KsATP		0.039		✓
PFK_g_KmADP	PFK_g_KmADP		1.000		✓
PFK_g_Ki2	PFK_g_Ki2		10.700		✓

6.4 Reaction GlcT_g

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

Name GlcT_g

Reaction equation



Reactant

Table 17: Properties of each reactant.

Id	Name	SBO
Glc_c	Glc_c	

Modifiers

Table 18: Properties of each modifier.

Id	Name	SBO
Glc_c	Glc_c	

Id	Name	SBO
Glc_g	Glc_g	
Glc_c	Glc_c	
Glc_g	Glc_g	

Product

Table 19: Properties of each product.

Id	Name	SBO
Glc_g	Glc_g	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \text{mass_action_rev}(\text{GlcT_g_k1}, [\text{Glc_c}], \text{GlcT_g_k2}, [\text{Glc_g}]) \quad (16)$$

$$\text{mass_action_rev}(k1, S, k2, P) = k1 \cdot S - k2 \cdot P \quad (17)$$

Table 20: Properties of each parameter.

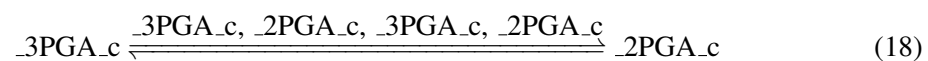
Id	Name	SBO	Value	Unit	Constant
GlcT_g_k1	GlcT_g_k1		250000.0		<input checked="" type="checkbox"/>
GlcT_g_k2	GlcT_g_k2		250000.0		<input checked="" type="checkbox"/>

6.5 Reaction PGAM_c

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

Name PGAM_c

Reaction equation



Reactant

Table 21: Properties of each reactant.

Id	Name	SBO
_3PGA_c	_3PGA_c	

Modifiers

Table 22: Properties of each modifier.

Id	Name	SBO
_3PGA_c	_3PGA_c	
_2PGA_c	_2PGA_c	
_3PGA_c	_3PGA_c	
_2PGA_c	_2PGA_c	

Product

Table 23: Properties of each product.

Id	Name	SBO
_2PGA_c	_2PGA_c	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = v1sub1prod(PGAM_c_Vmax, PGAM_c_Keq, [_3PGA_c], PGAM_c_Km3PGA, [_2PGA_c], PGAM_c_Km2PGA) \quad (19)$$

$$v1sub1prod(Vfmax, Keq, S, Ks, P, Kp) = \frac{Vfmax \cdot S \cdot \left(1 - \frac{P}{Keq \cdot S}\right)}{Ks \cdot \left(1 + \frac{S}{Ks} + \frac{P}{Kp}\right)} \quad (20)$$

Table 24: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
PGAM_c_Vmax	PGAM_c_Vmax		225.00		✓
PGAM_c_Keq	PGAM_c_Keq		0.17		✓
PGAM_c-_Km3PGA	PGAM_c-_Km3PGA		0.15		✓

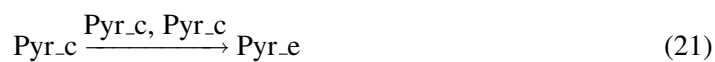
Id	Name	SBO	Value	Unit	Constant
PGAM_c- _Km2PGA	PGAM_c- _Km2PGA		0.16		<input checked="" type="checkbox"/>

6.6 Reaction PyrT_c

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

Name PyrT_c

Reaction equation



Reactant

Table 25: Properties of each reactant.

Id	Name	SBO
Pyr_c	Pyr_c	

Modifiers

Table 26: Properties of each modifier.

Id	Name	SBO
Pyr_c	Pyr_c	
Pyr_c	Pyr_c	

Product

Table 27: Properties of each product.

Id	Name	SBO
Pyr_e	Pyr_e	

Kinetic Law

Derived unit contains undeclared units

$$v_6 = v1_{\text{sub}}(\text{PyrT}_c_V_{\text{max}}, [\text{Pyr}_c], \text{PyrT}_c_K_{\text{mPyr}}) \quad (22)$$

$$v_{\text{sub}}(V_{\text{fmax}}, S, K_s) = \frac{V_{\text{fmax}} \cdot S}{K_s \cdot \left(1 + \frac{S}{K_s}\right)} \quad (23)$$

Table 28: Properties of each parameter.

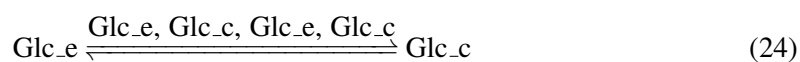
Id	Name	SBO	Value	Unit	Constant
PyrT_c_Vmax	PyrT_c_Vmax		230.00		<input checked="" type="checkbox"/>
PyrT_c_KmPyr	PyrT_c_KmPyr		1.96		<input checked="" type="checkbox"/>

6.7 Reaction GlcT_c

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

Name GlcT_c

Reaction equation



Reactant

Table 29: Properties of each reactant.

Id	Name	SBO
Glc_e	Glc_e	

Modifiers

Table 30: Properties of each modifier.

Id	Name	SBO
Glc_e	Glc_e	
Glc_c	Glc_c	
Glc_e	Glc_e	
Glc_c	Glc_c	

Product

Table 31: Properties of each product.

Id	Name	SBO
Glc_c	Glc_c	

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \frac{\text{GlcT_c_Vmax} \cdot ([\text{Glc_e}] - [\text{Glc_c}])}{\text{GlcT_c_KmGlc} + [\text{Glc_e}] + [\text{Glc_c}] + \frac{\text{GlcT_c_alpha} \cdot [\text{Glc_e}] \cdot [\text{Glc_c}]}{\text{GlcT_c_KmGlc}}} \quad (25)$$

Table 32: Properties of each parameter.

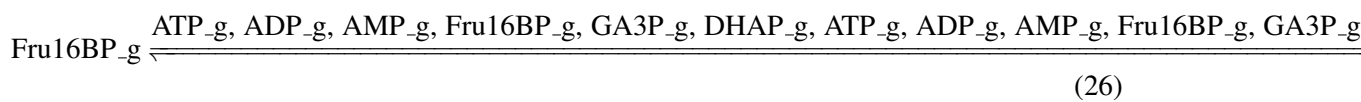
Id	Name	SBO	Value	Unit	Constant
GlcT_c_Vmax	GlcT_c_Vmax		111.70		✓
GlcT_c_KmGlc	GlcT_c_KmGlc		1.00		✓
GlcT_c_alpha	GlcT_c_alpha		0.75		✓

6.8 Reaction ALD_g

This is a reversible reaction of one reactant forming two products influenced by 15 modifiers.

Name ALD_g

Reaction equation



Reactant

Table 33: Properties of each reactant.

Id	Name	SBO
Fru16BP_g	Fru16BP_g	

Modifiers

Table 34: Properties of each modifier.

Id	Name	SBO
ATP_g	ATP_g	
ADP_g	ADP_g	
AMP_g	AMP_g	
Fru16BP_g	Fru16BP_g	
GA3P_g	GA3P_g	
DHAP_g	DHAP_g	
ATP_g	ATP_g	
ADP_g	ADP_g	
AMP_g	AMP_g	
Fru16BP_g	Fru16BP_g	
GA3P_g	GA3P_g	
DHAP_g	DHAP_g	
ATP_g	ATP_g	
ADP_g	ADP_g	
AMP_g	AMP_g	

Products

Table 35: Properties of each product.

Id	Name	SBO
GA3P_g	GA3P_g	
DHAP_g	DHAP_g	

Kinetic Law

Derived unit contains undeclared units

v_8

(27)

$$= \frac{ALD_g_Vmax}{ALD_g_KmFru16BP \cdot \left(1 + \frac{[ATP_g]}{ALD_g_KiATP} + \frac{[ADP_g]}{ALD_g_KiADP} + \frac{[AMP_g]}{ALD_g_KiAMP}\right) \cdot \left(1 + \frac{[GA3P_g]}{ALD_g_KmGA3P} + \frac{[DHAP_g]}{ALD_g_KmDHAP} + \dots\right)}$$

Table 36: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
ALD_g_Vmax	ALD_g_Vmax		560.000		☑

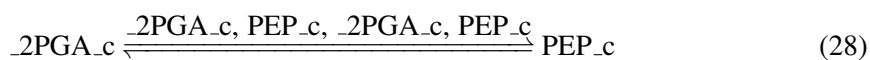
Id	Name	SBO	Value	Unit	Constant
ALD_g- _KmFru16BP	ALD_g- _KmFru16BP		0.009		✓
ALD_g_KiATP	ALD_g_KiATP		0.680		✓
ALD_g_KiADP	ALD_g_KiADP		1.510		✓
ALD_g_KiAMP	ALD_g_KiAMP		3.650		✓
ALD_g_Keq	ALD_g_Keq		0.084		✓
ALD_g_KmGA3P	ALD_g_KmGA3P		0.067		✓
ALD_g_KmDHAP	ALD_g_KmDHAP		0.015		✓
ALD_g_KiGA3P	ALD_g_KiGA3P		0.098		✓

6.9 Reaction ENO_c

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

Name ENO_c

Reaction equation



Reactant

Table 37: Properties of each reactant.

Id	Name	SBO
_2PGA_c	_2PGA_c	

Modifiers

Table 38: Properties of each modifier.

Id	Name	SBO
_2PGA_c	_2PGA_c	
PEP_c	PEP_c	
_2PGA_c	_2PGA_c	
PEP_c	PEP_c	

Product

Table 39: Properties of each product.

Id	Name	SBO
PEP_c	PEP_c	

Kinetic Law

Derived unit contains undeclared units

$$v_9 = v1sub1prod(ENO_c_Vmax, ENO_c_K_{eq}, [_2PGA_c], ENO_c_K_{m2PGA}, [PEP_c], ENO_c_K_{mPEP}) \quad (29)$$

$$v1sub1prod(Vfmax, Keq, S, Ks, P, Kp) = \frac{Vfmax \cdot S \cdot \left(1 - \frac{P}{K_{eq} \cdot S}\right)}{Ks \cdot \left(1 + \frac{S}{Ks} + \frac{P}{Kp}\right)} \quad (30)$$

Table 40: Properties of each parameter.

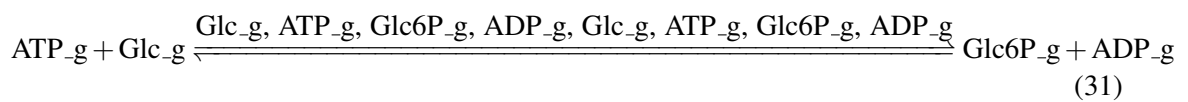
Id	Name	SBO	Value	Unit	Constant
ENO_c_Vmax	ENO_c_Vmax		598.000		✓
ENO_c_Keq	ENO_c_Keq		4.170		✓
ENO_c_Km2PGA	ENO_c_Km2PGA		0.054		✓
ENO_c_KmPEP	ENO_c_KmPEP		0.240		✓

6.10 Reaction HXK_g

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

Name HXK_g

Reaction equation



Reactants

Table 41: Properties of each reactant.

Id	Name	SBO
ATP_g	ATP_g	
Glc_g	Glc_g	

Modifiers

Table 42: Properties of each modifier.

Id	Name	SBO
Glc_g	Glc_g	
ATP_g	ATP_g	
Glc6P_g	Glc6P_g	
ADP_g	ADP_g	
Glc_g	Glc_g	
ATP_g	ATP_g	
Glc6P_g	Glc6P_g	
ADP_g	ADP_g	

Products

Table 43: Properties of each product.

Id	Name	SBO
Glc6P_g	Glc6P_g	
ADP_g	ADP_g	

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = v_{\text{sub2prod}}(\text{HXK_g_Vmax}, \text{HXK_g_Keq}, [\text{Glc_g}], \text{HXK_g_KmGlc}, [\text{ATP_g}], \text{HXK_g_KmATP}, [\text{Glc6P_g}], \text{HXK_g_KmGlc6P}, [\text{ADP_g}], \text{HXK_g_KmADP}) \quad (32)$$

$$v_{\text{sub2prod}}(\text{Vfmax}, \text{Keq}, \text{S1}, \text{Ks1}, \text{S2}, \text{Ks2}, \text{P1}, \text{Kp1}, \text{P2}, \text{Kp2}) = \frac{\text{Vfmax} \cdot \text{S1} \cdot \text{S2} \cdot \left(1 - \frac{\text{P1} \cdot \text{P2}}{\text{Keq} \cdot \text{S1} \cdot \text{S2}}\right)}{\text{Ks1} \cdot \text{Ks2} \cdot \left(1 + \frac{\text{S1}}{\text{Ks1}} + \frac{\text{P1}}{\text{Kp1}}\right) \cdot \left(1 + \frac{\text{S2}}{\text{Ks2}} + \frac{\text{P2}}{\text{Kp2}}\right)} \quad (33)$$

Table 44: Properties of each parameter.

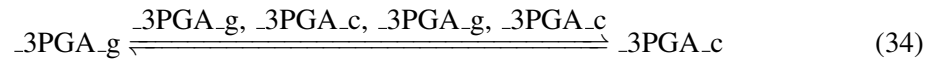
Id	Name	SBO	Value	Unit	Constant
HXX_g_Vmax	HXX_g_Vmax		1774.680		✓
HXX_g_Keq	HXX_g_Keq		759.000		✓
HXX_g_KmGlc	HXX_g_KmGlc		0.100		✓
HXX_g_KmATP	HXX_g_KmATP		0.116		✓
HXX_g_KmGlc6P	HXX_g_KmGlc6P		12.000		✓
HXX_g_KmADP	HXX_g_KmADP		0.126		✓

6.11 Reaction _3PGAT_g

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

Name _3PGAT_g

Reaction equation



Reactant

Table 45: Properties of each reactant.

Id	Name	SBO
_3PGA_g	_3PGA_g	

Modifiers

Table 46: Properties of each modifier.

Id	Name	SBO
_3PGA_g	_3PGA_g	
_3PGA_c	_3PGA_c	
_3PGA_g	_3PGA_g	
_3PGA_c	_3PGA_c	

Product

Table 47: Properties of each product.

Id	Name	SBO
_3PGA_c	_3PGA_c	

Kinetic Law

Derived unit contains undeclared units

$$v_{11} = \text{mass_action_rev}(_3\text{PGAT_g_k}, [_3\text{PGA_g}], _3\text{PGAT_g_k}, [_3\text{PGA_c}]) \quad (35)$$

$$\text{mass_action_rev}(k_1, S, k_2, P) = k_1 \cdot S - k_2 \cdot P \quad (36)$$

Table 48: Properties of each parameter.

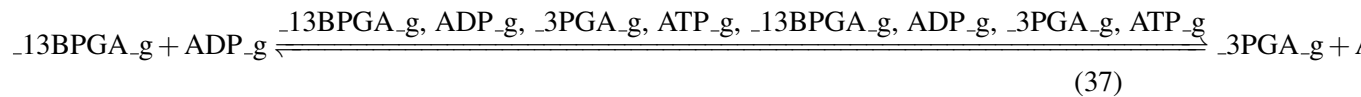
Id	Name	SBO	Value	Unit	Constant
_3PGAT_g_k	_3PGAT_g_k		250.0		<input checked="" type="checkbox"/>

6.12 Reaction PGK_g

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

Name PGK_g

Reaction equation



Reactants

Table 49: Properties of each reactant.

Id	Name	SBO
_13BPGA_g	_13BPGA_g	
ADP_g	ADP_g	

Modifiers

Table 50: Properties of each modifier.

Id	Name	SBO
_13BPGA_g	_13BPGA_g	
ADP_g	ADP_g	
_3PGA_g	_3PGA_g	
ATP_g	ATP_g	
_13BPGA_g	_13BPGA_g	
ADP_g	ADP_g	
_3PGA_g	_3PGA_g	
ATP_g	ATP_g	

Products

Table 51: Properties of each product.

Id	Name	SBO
_3PGA_g	_3PGA_g	
ATP_g	ATP_g	

Kinetic Law

Derived unit contains undeclared units

$$v_{12} = v_{\text{sub2prod}}(\text{PGK_g_Vmax}, \text{PGK_g_Keq}, [_{13}\text{BPGA_g}], \text{PGK_g_Km13BPGA}, [\text{ADP_g}], \text{PGK_g_KmADP}, [_{3}\text{PGA_g}], \text{PGK_g_Km3PGA}, [\text{ATP_g}], \text{PGK_g_KmATP}) \quad (38)$$

$$v_{\text{sub2prod}}(\text{Vfmax}, \text{Keq}, \text{S1}, \text{Ks1}, \text{S2}, \text{Ks2}, \text{P1}, \text{Kp1}, \text{P2}, \text{Kp2}) = \frac{\text{Vfmax} \cdot \text{S1} \cdot \text{S2} \cdot \left(1 - \frac{\text{P1} \cdot \text{P2}}{\text{Keq} \cdot \text{S1} \cdot \text{S2}}\right)}{\text{Ks1} \cdot \text{Ks2} \cdot \left(1 + \frac{\text{S1}}{\text{Ks1}} + \frac{\text{P1}}{\text{Kp1}}\right) \cdot \left(1 + \frac{\text{S2}}{\text{Ks2}} + \frac{\text{P2}}{\text{Kp2}}\right)} \quad (39)$$

Table 52: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
PGK_g_Vmax	PGK_g_Vmax		2862.000		✓
PGK_g_Keq	PGK_g_Keq		3377.000		✓
PGK_g-_Km13BPGA	PGK_g-_Km13BPGA		0.003		✓

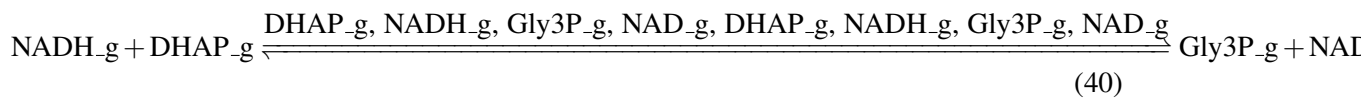
Id	Name	SBO	Value	Unit	Constant
PGK_g_KmADP	PGK_g_KmADP		0.100		<input checked="" type="checkbox"/>
PGK_g_Km3PGA	PGK_g_Km3PGA		1.620		<input checked="" type="checkbox"/>
PGK_g_KmATP	PGK_g_KmATP		0.290		<input checked="" type="checkbox"/>

6.13 Reaction G3PDH_g

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

Name G3PDH_g

Reaction equation



Reactants

Table 53: Properties of each reactant.

Id	Name	SBO
NADH_g	NADH_g	
DHAP_g	DHAP_g	

Modifiers

Table 54: Properties of each modifier.

Id	Name	SBO
DHAP_g	DHAP_g	
NADH_g	NADH_g	
Gly3P_g	Gly3P_g	
NAD_g	NAD_g	
DHAP_g	DHAP_g	
NADH_g	NADH_g	
Gly3P_g	Gly3P_g	
NAD_g	NAD_g	

Products

Table 55: Properties of each product.

Id	Name	SBO
Gly3P_g	Gly3P_g	
NAD_g	NAD_g	

Kinetic Law

Derived unit contains undeclared units

$$v_{13} = v_{2\text{sub}2\text{prod}}(\text{G3PDH_g_Vmax}, \text{G3PDH_g_Keq}, [\text{DHAP_g}], \text{G3PDH_g_KmDHAP}, [\text{NADH_g}], \text{G3PDH_g_KmNADH}, [\text{Gly3P_g}], \text{G3PDH_g_KmGly3P}, [\text{NAD_g}], \text{G3PDH_g_KmNAD}) \quad (41)$$

$$v_{2\text{sub}2\text{prod}}(\text{Vfmax}, \text{Keq}, \text{S1}, \text{Ks1}, \text{S2}, \text{Ks2}, \text{P1}, \text{Kp1}, \text{P2}, \text{Kp2}) = \frac{\text{Vfmax} \cdot \text{S1} \cdot \text{S2} \cdot \left(1 - \frac{\text{P1} \cdot \text{P2}}{\text{Keq} \cdot \text{S1} \cdot \text{S2}}\right)}{\text{Ks1} \cdot \text{Ks2} \cdot \left(1 + \frac{\text{S1}}{\text{Ks1}} + \frac{\text{P1}}{\text{Kp1}}\right) \cdot \left(1 + \frac{\text{S2}}{\text{Ks2}} + \frac{\text{P2}}{\text{Kp2}}\right)} \quad (42)$$

Table 56: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
G3PDH_g_Vmax	G3PDH_g_Vmax		465.00		✓
G3PDH_g_Keq	G3PDH_g_Keq		17085.00		✓
G3PDH_g_KmDHAP	G3PDH_g_KmDHAP		0.10		✓
G3PDH_g_KmNADH	G3PDH_g_KmNADH		0.01		✓
G3PDH_g_KmGly3P	G3PDH_g_KmGly3P		2.00		✓
G3PDH_g_KmNAD	G3PDH_g_KmNAD		0.40		✓

6.14 Reaction GPO_c

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

Name GPO_c

Reaction equation



Reactant

Table 57: Properties of each reactant.

Id	Name	SBO
Gly3P_c	Gly3P_c	

Modifiers

Table 58: Properties of each modifier.

Id	Name	SBO
Gly3P_c	Gly3P_c	
Gly3P_c	Gly3P_c	

Product

Table 59: Properties of each product.

Id	Name	SBO
DHAP_c	DHAP_c	

Kinetic Law

Derived unit contains undeclared units

$$v_{14} = v_{\text{sub}}(\text{GPO}_c\text{-Vmax}, [\text{Gly3P}_c], \text{GPO}_c\text{-KmGly3P}) \quad (44)$$

$$v_{\text{sub}}(\text{Vfmax}, S, K_s) = \frac{\text{Vfmax} \cdot S}{K_s \cdot \left(1 + \frac{S}{K_s}\right)} \quad (45)$$

Table 60: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
GPO_c-Vmax	GPO_c-Vmax		368.0		✓
GPO_c-KmGly3P	GPO_c-KmGly3P		1.7		✓

6.15 Reaction ATPu_c

This is an irreversible reaction of one reactant forming one product influenced by four modifiers.

Name ATPu_c

Reaction equation



Reactant

Table 61: Properties of each reactant.

Id	Name	SBO
ATP_c	ATP_c	

Modifiers

Table 62: Properties of each modifier.

Id	Name	SBO
ATP_c	ATP_c	
ADP_c	ADP_c	
ATP_c	ATP_c	
ADP_c	ADP_c	

Product

Table 63: Properties of each product.

Id	Name	SBO
ADP_c	ADP_c	

Kinetic Law

Derived unit contains undeclared units

$$v_{15} = \frac{\text{ATPu_c_k} \cdot [\text{ATP_c}]}{[\text{ADP_c}]} \quad (47)$$

Table 64: Properties of each parameter.

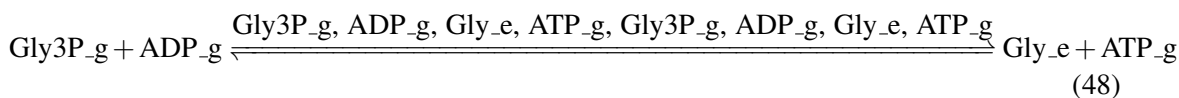
Id	Name	SBO	Value	Unit	Constant
ATPu_c_k	ATPu_c_k		50.0		<input checked="" type="checkbox"/>

6.16 Reaction GK_g

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

Name GK_g

Reaction equation



Reactants

Table 65: Properties of each reactant.

Id	Name	SBO
Gly3P_g	Gly3P_g	
ADP_g	ADP_g	

Modifiers

Table 66: Properties of each modifier.

Id	Name	SBO
Gly3P_g	Gly3P_g	
ADP_g	ADP_g	
Gly_e	Gly_e	
ATP_g	ATP_g	
Gly3P_g	Gly3P_g	
ADP_g	ADP_g	
Gly_e	Gly_e	
ATP_g	ATP_g	

Products

Table 67: Properties of each product.

Id	Name	SBO
Gly_e	Gly_e	
ATP_g	ATP_g	

Kinetic Law

Derived unit contains undeclared units

$$v_{16} = v_{\text{sub2prod}}(\text{GK_g_Vmax}, \text{GK_g_Keq}, [\text{Gly3P_g}], \text{GK_g_KmGly3P}, [\text{ADP_g}], \text{GK_g_KmADP}, [\text{Gly_e}], \text{GK_g_KmGly}, [\text{ATP_g}], \text{GK_g_KmATP}) \quad (49)$$

$$v_{\text{sub2prod}}(\text{Vfmax}, \text{Keq}, \text{S1}, \text{Ks1}, \text{S2}, \text{Ks2}, \text{P1}, \text{Kp1}, \text{P2}, \text{Kp2}) = \frac{\text{Vfmax} \cdot \text{S1} \cdot \text{S2} \cdot \left(1 - \frac{\text{P1} \cdot \text{P2}}{\text{Keq} \cdot \text{S1} \cdot \text{S2}}\right)}{\text{Ks1} \cdot \text{Ks2} \cdot \left(1 + \frac{\text{S1}}{\text{Ks1}} + \frac{\text{P1}}{\text{Kp1}}\right) \cdot \left(1 + \frac{\text{S2}}{\text{Ks2}} + \frac{\text{P2}}{\text{Kp2}}\right)} \quad (50)$$

Table 68: Properties of each parameter.

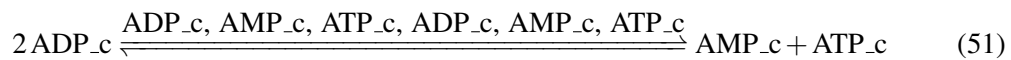
Id	Name	SBO	Value	Unit	Constant
GK_g_Vmax	GK_g_Vmax		200.000		✓
GK_g_Keq	GK_g_Keq		$8.37 \cdot 10^{-4}$		✓
GK_g_KmGly3P	GK_g_KmGly3P		3.830		✓
GK_g_KmADP	GK_g_KmADP		0.560		✓
GK_g_KmGly	GK_g_KmGly		0.440		✓
GK_g_KmATP	GK_g_KmATP		0.240		✓

6.17 Reaction AK_c

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

Name AK_c

Reaction equation



Reactant

Table 69: Properties of each reactant.

Id	Name	SBO
ADP_c	ADP_c	

Modifiers

Table 70: Properties of each modifier.

Id	Name	SBO
ADP_c	ADP_c	
AMP_c	AMP_c	
ATP_c	ATP_c	
ADP_c	ADP_c	
AMP_c	AMP_c	
ATP_c	ATP_c	

Products

Table 71: Properties of each product.

Id	Name	SBO
AMP_c	AMP_c	
ATP_c	ATP_c	

Kinetic Law

Derived unit contains undeclared units

$$v_{17} = v_{AK}([ADP_c], [AMP_c], [ATP_c], AK_c.k1, AK_c.k2) \quad (52)$$

$$v_{AK}(ADP, AMP, ATP, k1, k2) = k1 \cdot ADP^2 - AMP \cdot ATP \cdot k2 \quad (53)$$

Table 72: Properties of each parameter.

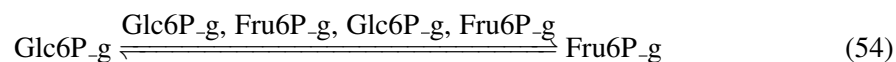
Id	Name	SBO	Value	Unit	Constant
AK_c.k1	AK_c.k1		480.0		<input checked="" type="checkbox"/>
AK_c.k2	AK_c.k2		1000.0		<input checked="" type="checkbox"/>

6.18 Reaction PGI_g

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

Name PGI_g

Reaction equation



Reactant

Table 73: Properties of each reactant.

Id	Name	SBO
Glc6P_g	Glc6P_g	

Modifiers

Table 74: Properties of each modifier.

Id	Name	SBO
Glc6P_g	Glc6P_g	
Fru6P_g	Fru6P_g	
Glc6P_g	Glc6P_g	
Fru6P_g	Fru6P_g	

Product

Table 75: Properties of each product.

Id	Name	SBO
Fru6P_g	Fru6P_g	

Kinetic Law

Derived unit contains undeclared units

$$v_{18} = \frac{\text{PGI}_g \cdot V_{\max} \cdot [\text{Glc6P}_g] \cdot \left(1 - \frac{[\text{Fru6P}_g]}{\text{PGI}_g \cdot K_{\text{eq}} \cdot [\text{Glc6P}_g]}\right)}{\text{PGI}_g \cdot K_{\text{mGlc6P}} \cdot \left(1 + \frac{[\text{Glc6P}_g]}{\text{PGI}_g \cdot K_{\text{mGlc6P}}} + \frac{[\text{Fru6P}_g]}{\text{PGI}_g \cdot K_{\text{mFru6P}}} + \frac{[\text{6PG}_g]}{\text{PGI}_g \cdot K_{\text{i6PG}}}\right)} \quad (55)$$

Table 76: Properties of each parameter.

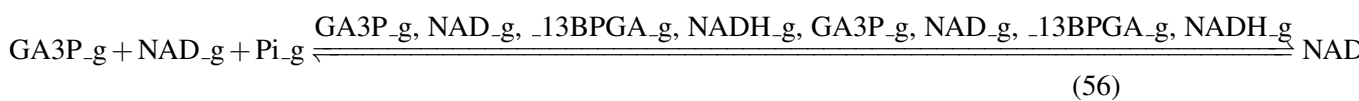
Id	Name	SBO	Value	Unit	Constant
PGI_g_Vmax	PGI_g_Vmax		1305.000		✓
PGI_g-_KmGlc6P	PGI_g_KmGlc6P		0.400		✓
PGI_g_Keq	PGI_g_Keq		0.457		✓
PGI_g-_KmFru6P	PGI_g_KmFru6P		0.120		✓
_6PG_g	_6PG_g		0.084		✓
PGI_g_Ki6PG	PGI_g_Ki6PG		0.140		✓

6.19 Reaction GAPDH_g

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

Name GAPDH_g

Reaction equation



Reactants

Table 77: Properties of each reactant.

Id	Name	SBO
GA3P_g	GA3P_g	
NAD_g	NAD_g	
Pi_g	Pi_g	

Modifiers

Table 78: Properties of each modifier.

Id	Name	SBO
GA3P_g	GA3P_g	
NAD_g	NAD_g	
_13BPGA_g	_13BPGA_g	
NADH_g	NADH_g	

Id	Name	SBO
GA3P_g	GA3P_g	
NAD_g	NAD_g	
_13BPGA_g	_13BPGA_g	
NADH_g	NADH_g	

Products

Table 79: Properties of each product.

Id	Name	SBO
NADH_g	NADH_g	
_13BPGA_g	_13BPGA_g	

Kinetic Law

Derived unit contains undeclared units

$$v_{19} = v_{2\text{sub}2\text{prod}}(\text{GAPDH_g_Vmax}, \text{GAPDH_g_Keq}, [\text{GA3P_g}], \text{GAPDH_g_KmGA3P}, [\text{NAD_g}], \text{GAPDH_g_KmNAD}, [_{13}\text{BPGA_g}], \text{GAPDH_g_Km13BPGA}, [\text{NADH_g}], \text{GAPDH_g_KmNADH}) \quad (57)$$

$$v_{2\text{sub}2\text{prod}}(\text{Vfmax}, \text{Keq}, \text{S1}, \text{Ks1}, \text{S2}, \text{Ks2}, \text{P1}, \text{Kp1}, \text{P2}, \text{Kp2}) = \frac{\text{Vfmax} \cdot \text{S1} \cdot \text{S2} \cdot \left(1 - \frac{\text{P1} \cdot \text{P2}}{\text{Keq} \cdot \text{S1} \cdot \text{S2}}\right)}{\text{Ks1} \cdot \text{Ks2} \cdot \left(1 + \frac{\text{S1}}{\text{Ks1}} + \frac{\text{P1}}{\text{Kp1}}\right) \cdot \left(1 + \frac{\text{S2}}{\text{Ks2}} + \frac{\text{P2}}{\text{Kp2}}\right)} \quad (58)$$

Table 80: Properties of each parameter.

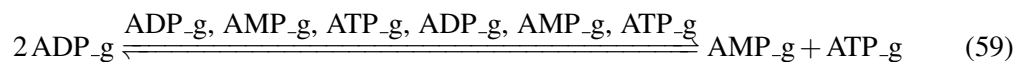
Id	Name	SBO	Value	Unit	Constant
GAPDH_g_Vmax	GAPDH_g_Vmax		720.900		✓
GAPDH_g_Keq	GAPDH_g_Keq		0.066		✓
GAPDH_g-_KmGA3P	GAPDH_g-_KmGA3P		0.150		✓
GAPDH_g-_KmNAD	GAPDH_g-_KmNAD		0.450		✓
GAPDH_g-_Km13BPGA	GAPDH_g-_Km13BPGA		0.100		✓
GAPDH_g-_KmNADH	GAPDH_g-_KmNADH		0.020		✓

6.20 Reaction AK_g

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

Name AK_g

Reaction equation



Reactant

Table 81: Properties of each reactant.

Id	Name	SBO
ADP_g	ADP_g	

Modifiers

Table 82: Properties of each modifier.

Id	Name	SBO
ADP_g	ADP_g	
AMP_g	AMP_g	
ATP_g	ATP_g	
ADP_g	ADP_g	
AMP_g	AMP_g	
ATP_g	ATP_g	

Products

Table 83: Properties of each product.

Id	Name	SBO
AMP_g	AMP_g	
ATP_g	ATP_g	

Kinetic Law

Derived unit contains undeclared units

$$v_{20} = v_{AK}([ADP_g], [AMP_g], [ATP_g], AK_g_k1, AK_g_k2) \quad (60)$$

$$v_{AK}(ADP, AMP, ATP, k1, k2) = k1 \cdot ADP^2 - AMP \cdot ATP \cdot k2 \quad (61)$$

Table 84: Properties of each parameter.

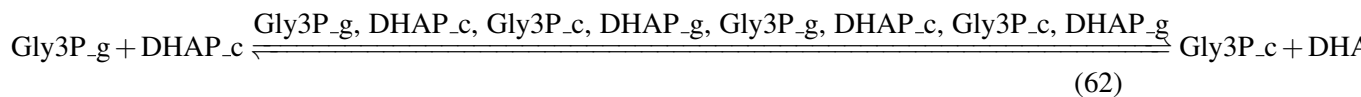
Id	Name	SBO	Value	Unit	Constant
AK_g_k1	AK_g_k1		480.0		<input checked="" type="checkbox"/>
AK_g_k2	AK_g_k2		1000.0		<input checked="" type="checkbox"/>

6.21 Reaction GDA_g

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

Name GDA_g

Reaction equation



Reactants

Table 85: Properties of each reactant.

Id	Name	SBO
Gly3P_g	Gly3P_g	
DHAP_c	DHAP_c	

Modifiers

Table 86: Properties of each modifier.

Id	Name	SBO
Gly3P_g	Gly3P_g	
DHAP_c	DHAP_c	
Gly3P_c	Gly3P_c	
DHAP_g	DHAP_g	
Gly3P_g	Gly3P_g	
DHAP_c	DHAP_c	
Gly3P_c	Gly3P_c	
DHAP_g	DHAP_g	

Products

Table 87: Properties of each product.

Id	Name	SBO
Gly3P_c	Gly3P_c	
DHAP_g	DHAP_g	

Kinetic Law

Derived unit contains undeclared units

$$v_{21} = [\text{Gly3P}_g] \cdot \text{GDA}_g\text{-k} \cdot [\text{DHAP}_c] - [\text{Gly3P}_c] \cdot \text{GDA}_g\text{-k} \cdot [\text{DHAP}_g] \quad (63)$$

Table 88: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
GDA_g_k	GDA_g_k		600.0		<input checked="" type="checkbox"/>

7 Derived Rate Equations

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

Identifiers for kinetic laws highlighted in gray cannot be verified to evaluate to units of SBML substance per time. As a result, some SBML interpreters may not be able to verify the consistency of the units on quantities in the model. Please check if

- parameters without an unit definition are involved or
- volume correction is necessary because the `hasOnlySubstanceUnits` flag may be set to `false` and `spacialDimensions` > 0 for certain species.

7.1 Species `_2PGA_c`

Name `_2PGA_c`

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

This species takes part in six reactions (as a reactant in `ENO_c` and as a product in `PGAM_c` and as a modifier in `PGAM_c`, `PGAM_c`, `ENO_c`, `ENO_c`).

$$\frac{d}{dt} \text{_2PGA_c} = v_5 - v_9 \quad (64)$$

7.2 Species DHAP_c

Name DHAP_c

Initial concentration 2.23132912 nmol · μl⁻¹

This species takes part in four reactions (as a reactant in [GDA_g](#) and as a product in [GPO_c](#) and as a modifier in [GDA_g](#), [GDA_g](#)).

$$\frac{d}{dt}\text{DHAP}_c = v_{14} - v_{21} \quad (65)$$

7.3 Species ATP_g

Name ATP_g

Initial concentration 0.2405 nmol · μl⁻¹

This species takes part in 18 reactions (as a reactant in [PFK_g](#), [HXK_g](#) and as a product in [PGK_g](#), [GK_g](#), [AK_g](#) and as a modifier in [PFK_g](#), [PFK_g](#), [ALD_g](#), [ALD_g](#), [ALD_g](#), [HXK_g](#), [HXK_g](#), [PGK_g](#), [PGK_g](#), [GK_g](#), [GK_g](#), [AK_g](#), [AK_g](#)).

$$\frac{d}{dt}\text{ATP}_g = v_{12} + v_{16} + v_{20} - v_3 - v_{10} \quad (66)$$

7.4 Species DHAP_g

Name DHAP_g

Initial concentration 8.483130623 nmol · μl⁻¹

This species takes part in twelve reactions (as a reactant in [TPI_g](#), [G3PDH_g](#) and as a product in [ALD_g](#), [GDA_g](#) and as a modifier in [TPI_g](#), [TPI_g](#), [ALD_g](#), [ALD_g](#), [G3PDH_g](#), [G3PDH_g](#), [GDA_g](#), [GDA_g](#)).

$$\frac{d}{dt}\text{DHAP}_g = v_8 + v_{21} - v_1 - v_{13} \quad (67)$$

7.5 Species ADP_g

Name ADP_g

Initial concentration 1.519 nmol · μl⁻¹

This species takes part in 18 reactions (as a reactant in [PGK_g](#), [GK_g](#), [AK_g](#) and as a product in [PFK_g](#), [HXK_g](#) and as a modifier in [PFK_g](#), [PFK_g](#), [ALD_g](#), [ALD_g](#), [ALD_g](#), [HXK_g](#), [HXK_g](#), [PGK_g](#), [PGK_g](#), [GK_g](#), [GK_g](#), [AK_g](#), [AK_g](#)).

$$\frac{d}{dt}\text{ADP}_g = v_3 + v_{10} - v_{12} - v_{16} - 2 v_{20} \quad (68)$$

7.6 Species Glc6P_g

Name Glc6P_g

Initial concentration $0.5 \text{ nmol} \cdot \mu\text{l}^{-1}$

This species takes part in six reactions (as a reactant in [PGI_g](#) and as a product in [HXK_g](#) and as a modifier in [HXK_g](#), [HXK_g](#), [PGI_g](#), [PGI_g](#)).

$$\frac{d}{dt}\text{Glc6P}_g = v_{10} - v_{18} \quad (69)$$

7.7 Species ADP_c

Name ADP_c

Initial concentration $1.3165 \text{ nmol} \cdot \mu\text{l}^{-1}$

This species takes part in nine reactions (as a reactant in [PYK_c](#), [AK_c](#) and as a product in [ATPu_c](#) and as a modifier in [PYK_c](#), [PYK_c](#), [ATPu_c](#), [ATPu_c](#), [AK_c](#), [AK_c](#)).

$$\frac{d}{dt}\text{ADP}_c = v_{15} - v_2 - 2 v_{17} \quad (70)$$

7.8 Species _3PGA_c

Name _3PGA_c

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

This species takes part in six reactions (as a reactant in [PGAM_c](#) and as a product in [_3PGAT_g](#) and as a modifier in [PGAM_c](#), [PGAM_c](#), [_3PGAT_g](#), [_3PGAT_g](#)).

$$\frac{d}{dt}_3\text{PGA}_c = v_{11} - v_5 \quad (71)$$

7.9 Species Fru6P_g

Name Fru6P_g

Initial concentration $0.5 \text{ nmol} \cdot \mu\text{l}^{-1}$

This species takes part in six reactions (as a reactant in [PFK_g](#) and as a product in [PGI_g](#) and as a modifier in [PFK_g](#), [PFK_g](#), [PGI_g](#), [PGI_g](#)).

$$\frac{d}{dt}\text{Fru6P}_g = v_{18} - v_3 \quad (72)$$

7.10 Species Pi_g

Name Pi_g

Initial concentration $0 \text{ nmol} \cdot \mu\text{l}^{-1}$

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

$$\frac{d}{dt}\text{Pi}_g = 0 \quad (73)$$

7.11 Species O2_c

Name O2_c

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

$$\frac{d}{dt}\text{O2}_c = 0 \quad (74)$$

7.12 Species Gly_e

Name Gly_e

Initial concentration $0 \text{ nmol} \cdot \mu\text{l}^{-1}$

This species takes part in three reactions (as a product in [GK_g](#) and as a modifier in [GK_g](#), [GK_g](#)), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt}\text{Gly}_e = 0 \quad (75)$$

7.13 Species ATP_c

Name ATP_c

Initial concentration $0.3417 \text{ nmol} \cdot \mu\text{l}^{-1}$

This species takes part in nine reactions (as a reactant in [ATPu_c](#) and as a product in [PYK_c](#), [AK_c](#) and as a modifier in [PYK_c](#), [PYK_c](#), [ATPu_c](#), [ATPu_c](#), [AK_c](#), [AK_c](#)).

$$\frac{d}{dt}\text{ATP}_c = v_2 + v_{17} - v_{15} \quad (76)$$

7.14 Species `_13BPGA_g`

Name `_13BPGA_g`

Initial concentration $0.5 \text{ nmol} \cdot \mu\text{l}^{-1}$

This species takes part in six reactions (as a reactant in `PGK_g` and as a product in `GAPDH_g` and as a modifier in `PGK_g`, `PGK_g`, `GAPDH_g`, `GAPDH_g`).

$$\frac{d}{dt} \text{_13BPGA_g} = v_{19} - v_{12} \quad (77)$$

7.15 Species `Glc_c`

Name `Glc_c`

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

This species takes part in six reactions (as a reactant in `GlcT_g` and as a product in `GlcT_c` and as a modifier in `GlcT_g`, `GlcT_g`, `GlcT_c`, `GlcT_c`).

$$\frac{d}{dt} \text{Glc_c} = v_7 - v_4 \quad (78)$$

7.16 Species `Glc_e`

Name `Glc_e`

Initial concentration $5 \text{ nmol} \cdot \mu\text{l}^{-1}$

This species takes part in three reactions (as a reactant in `GlcT_c` and as a modifier in `GlcT_c`, `GlcT_c`), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{d}{dt} \text{Glc_e} = 0 \quad (79)$$

7.17 Species `Glc_g`

Name `Glc_g`

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

This species takes part in six reactions (as a reactant in `HXK_g` and as a product in `GlcT_g` and as a modifier in `GlcT_g`, `GlcT_g`, `HXK_g`, `HXK_g`).

$$\frac{d}{dt} \text{Glc_g} = v_4 - v_{10} \quad (80)$$

7.18 Species `Pyr_c`

Name `Pyr_c`

Initial concentration $10 \text{ nmol} \cdot \mu\text{l}^{-1}$

This species takes part in six reactions (as a reactant in `PyrT_c` and as a product in `PYK_c` and as a modifier in `PYK_c`, `PYK_c`, `PyrT_c`, `PyrT_c`).

$$\frac{d}{dt}\text{Pyr}_c = v_2 - v_6 \quad (81)$$

7.19 Species `Pyr_e`

Name `Pyr_e`

Initial concentration $0 \text{ nmol} \cdot \mu\text{l}^{-1}$

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

$$\frac{d}{dt}\text{Pyr}_e = 0 \quad (82)$$

7.20 Species `NAD_g`

Name `NAD_g`

Initial concentration $2 \text{ nmol} \cdot \mu\text{l}^{-1}$

This species takes part in six reactions (as a reactant in `GAPDH_g` and as a product in `G3PDH_g` and as a modifier in `G3PDH_g`, `G3PDH_g`, `GAPDH_g`, `GAPDH_g`).

$$\frac{d}{dt}\text{NAD}_g = v_{13} - v_{19} \quad (83)$$

7.21 Species `Fru16BP_g`

Name `Fru16BP_g`

Initial concentration $10 \text{ nmol} \cdot \mu\text{l}^{-1}$

This species takes part in six reactions (as a reactant in `ALD_g` and as a product in `PFK_g` and as a modifier in `PFK_g`, `PFK_g`, `ALD_g`, `ALD_g`).

$$\frac{d}{dt}\text{Fru16BP}_g = v_3 - v_8 \quad (84)$$

7.22 Species GA3P_g

Name GA3P_g

Initial concentration 2.5 nmol · μl⁻¹

This species takes part in nine reactions (as a reactant in GAPDH_g and as a product in TPI_g, ALD_g and as a modifier in TPI_g, TPI_g, ALD_g, ALD_g, GAPDH_g, GAPDH_g).

$$\frac{d}{dt}\text{GA3P}_g = v_1 + v_8 - v_{19} \quad (85)$$

7.23 Species CO2_c

Name CO2_c

Initial concentration 0 nmol · μl⁻¹

$$\frac{d}{dt}\text{CO2}_c = 0 \quad (86)$$

7.24 Species CO2_g

Name CO2_g

Initial concentration 0 nmol · μl⁻¹

$$\frac{d}{dt}\text{CO2}_g = 0 \quad (87)$$

7.25 Species Gly3P_c

Name Gly3P_c

Initial concentration 2.76867088 nmol · μl⁻¹

This species takes part in six reactions (as a reactant in GPO_c and as a product in GDA_g and as a modifier in GPO_c, GPO_c, GDA_g, GDA_g).

$$\frac{d}{dt}\text{Gly3P}_c = v_{21} - v_{14} \quad (88)$$

7.26 Species Gly3P_g

Name Gly3P_g

Initial concentration 10.51686938 nmol · μl⁻¹

This species takes part in nine reactions (as a reactant in GK_g, GDA_g and as a product in G3PDH_g and as a modifier in G3PDH_g, G3PDH_g, GK_g, GK_g, GDA_g, GDA_g).

$$\frac{d}{dt}\text{Gly3P}_g = v_{13} - v_{16} - v_{21} \quad (89)$$

7.27 Species PEP_c

Name PEP_c

Initial concentration 1 nmol · μl⁻¹

This species takes part in six reactions (as a reactant in [PYK_c](#) and as a product in [ENO_c](#) and as a modifier in [PYK_c](#), [PYK_c](#), [ENO_c](#), [ENO_c](#)).

$$\frac{d}{dt} \text{PEP}_c = v_9 - v_2 \quad (90)$$

7.28 Species AMP_g

Name AMP_g

Initial concentration 4.2405 nmol · μl⁻¹

This species takes part in six reactions (as a product in [AK_g](#) and as a modifier in [ALD_g](#), [ALD_g](#), [ALD_g](#), [AK_g](#), [AK_g](#)).

$$\frac{d}{dt} \text{AMP}_g = v_{20} \quad (91)$$

7.29 Species _3PGA_g

Name _3PGA_g

Initial concentration 0.1 nmol · μl⁻¹

This species takes part in six reactions (as a reactant in [_3PGAT_g](#) and as a product in [PGK_g](#) and as a modifier in [_3PGAT_g](#), [_3PGAT_g](#), [PGK_g](#), [PGK_g](#)).

$$\frac{d}{dt} \text{_3PGA}_g = v_{12} - v_{11} \quad (92)$$

7.30 Species AMP_c

Name AMP_c

Initial concentration 2.2418 nmol · μl⁻¹

This species takes part in three reactions (as a product in [AK_c](#) and as a modifier in [AK_c](#), [AK_c](#)).

$$\frac{d}{dt} \text{AMP}_c = v_{17} \quad (93)$$

7.31 Species NADH_g

Name NADH_g

Initial concentration 2 nmol · μl⁻¹

This species takes part in six reactions (as a reactant in G3PDH_g and as a product in GAPDH_g and as a modifier in G3PDH_g, G3PDH_g, GAPDH_g, GAPDH_g).

$$\frac{d}{dt}\text{NADH}_g = v_{19} - v_{13} \quad (94)$$

A Glossary of Systems Biology Ontology Terms

SBO:0000290 physical compartment: Specific location of space, that can be bounded or not.
A physical compartment can have 1, 2 or 3 dimensions

SBML²TeX was developed by Andreas Dräger^a, Hannes Planatscher^a, Dieudonné M Wouamba^a, Adrian Schröder^a, Michael Hucka^b, Lukas Endler^c, Martin Golebiewski^d and Andreas Zell^a. Please see <http://www.ra.cs.uni-tuebingen.de/software/SBML2LaTeX> for more information.

^aCenter for Bioinformatics Tübingen (ZBIT), Germany

^bCalifornia Institute of Technology, Beckman Institute BNMC, Pasadena, United States

^cEuropean Bioinformatics Institute, Wellcome Trust Genome Campus, Hinxton, United Kingdom

^dEML Research gGmbH, Heidelberg, Germany