SBML Model Report

Model name: “Kerkhoven2013 - Glycolysis and Pentose Phosphate Pathway in T.brucei - MODEL D (with ATP:ADP antiporter)”

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 Chelliah[1] and Eduard Kerkhoven[2] at February third 2014 at 10:23 a. m. and last time modified at March fifth 2014 at 3:55 p. m. Table 1 provides an overview of the quantities of all components of this model.

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

Element	Quantity	Element	Quantity
compartment types	0	compartments	3
species types	0	species	46
events	0	constraints	0
reactions	36	function definitions	7
global parameters	0	unit definitions	5
rules	0	initial assignments	0

Model Notes

Kerkhoven2013 - Glycolysis and Pentose Phosphate Pathway in T.brucei - MODEL D (with ATP:ADP antiporter)

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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 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 D 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: BIOMD0000000511 .

To cite BioModels Database, please use: BioModels Database: An enhanced, curated and annotated resourcefor published quantitative kinetic models .

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	☑	
`glycosome`	glycosome		3	0.2451	µl	☑	
`default`	default	0000290	3	1	litre	☑	

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

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

Table 3: Properties of each species.

Id	Name	Compartment	Derived Unit	Constant	Boundary Condition
_2PGA_c	_2PGA_c	cytosol	$\mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$	☐	☐
ATP_c	ATP_c	cytosol	$\mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$	☐	☐
DHAP_c	DHAP_c	cytosol	$\mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$	☐	☐
ATP_g	ATP_g	glycosome	$\mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$	☐	☐
DHAP_g	DHAP_g	glycosome	$\mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$	☐	☐
ADP_g	ADP_g	glycosome	$\mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$	☐	☐
Glc6P_g	Glc6P_g	glycosome	$\mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$	☐	☐
ADP_c	ADP_c	cytosol	$\mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$	☐	☐
_3PGA_c	_3PGA_c	cytosol	$\mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$	☐	☐
Fru6P_g	Fru6P_g	glycosome	$\mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$	☐	☐
Pi_g	Pi_g	glycosome	$\mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$	☑	☑
O2_c	O2_c	default	$\mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$	☑	☑
NADP_c	NADP_c	cytosol	$\mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$	☐	☐
NADP_g	NADP_g	glycosome	$\mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$	☐	☐
_6PG_g	_6PG_g	glycosome	$\mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$	☐	☐
CO2_c	CO2_c	cytosol	$\mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$	☑	☑
Ru5P_c	Ru5P_c	cytosol	$\mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$	☐	☐
_6PG_c	_6PG_c	cytosol	$\mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$	☐	☐
Ru5P_g	Ru5P_g	glycosome	$\mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$	☐	☐
Glc6P_c	Glc6P_c	cytosol	$\mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$	☐	☐
Rib5P_c	Rib5P_c	cytosol	$\mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$	☑	☑

Id	Name	Compartment	Derived Unit	Constant	Boundary Condition
_13BPGA_g	_13BPGA_g	glycosome	$\mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$	⊟	⊟
Glc_c	Glc_c	cytosol	$\mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$	⊟	⊟
Rib5P_g	Rib5P_g	glycosome	$\mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$	☑	☑
Glc_g	Glc_g	glycosome	$\mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$	⊟	⊟
Glc_e	Glc_e	default	$\mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$	☑	☑
NADPH_g	NADPH_g	glycosome	$\mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$	⊟	⊟
NADPH_c	NADPH_c	cytosol	$\mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$	⊟	⊟
Pyr_c	Pyr_c	cytosol	$\mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$	⊟	⊟
Pyr_e	Pyr_e	default	$\mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$	☑	☑
NAD_g	NAD_g	glycosome	$\mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$	⊟	⊟
Fru16BP_g	Fru16BP_g	glycosome	$\mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$	⊟	⊟
GA3P_g	GA3P_g	glycosome	$\mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$	⊟	⊟
Gly_e	Gly_e	default	$\mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$	☑	☑
TSH2_c	TSH2_c	cytosol	$\mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$	⊟	⊟
CO2_g	CO2_g	glycosome	$\mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$	☑	☑
Gly3P_c	Gly3P_c	cytosol	$\mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$	⊟	⊟
Gly3P_g	Gly3P_g	glycosome	$\mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$	⊟	⊟
_6PGL_c	_6PGL_c	cytosol	$\mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$	⊟	⊟
TS2_c	TS2_c	cytosol	$\mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$	⊟	⊟
_6PGL_g	_6PGL_g	glycosome	$\mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$	⊟	⊟
PEP_c	PEP_c	cytosol	$\mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$	⊟	⊟
AMP_g	AMP_g	glycosome	$\mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$	⊟	⊟
_3PGA_g	_3PGA_g	glycosome	$\mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$	⊟	⊟
AMP_c	AMP_c	cytosol	$\mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$	⊟	⊟
NADH_g	NADH_g	glycosome	$\mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$	⊟	⊟

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

$$k1 \cdot ADP^2 - AMP \cdot ATP \cdot k2 \tag{1}$$

5.2 Function definition v2sub2prod

Name v2sub2prod

Arguments Vfmax, Keq, S1, Ks1, S2, Ks2, P1, Kp1, P2, Kp2

Mathematical Expression

$$\frac{Vfmax \cdot S1 \cdot S2 \cdot \left(1 - \frac{P1 \cdot P2}{Keq \cdot S1 \cdot S2}\right)}{Ks1 \cdot Ks2 \cdot \left(1 + \frac{S1}{Ks1} + \frac{P1}{Kp1}\right) \cdot \left(1 + \frac{S2}{Ks2} + \frac{P2}{Kp2}\right)} \tag{2}$$

5.3 Function definition v1sub

Name v1sub

Arguments Vfmax, S, Ks

Mathematical Expression

$$\frac{Vfmax \cdot S}{Ks \cdot \left(1 + \frac{S}{Ks}\right)} \tag{3}$$

5.4 Function definition v2sub2prod_compinhib

Name v2sub2prod_compinhib

Arguments Vfmax, Keq, S1, Ks1, S2, Ks2, P1, Kp1, P2, Kp2, I1, Ki1, I2, Ki2

Mathematical Expression

$$\frac{Vfmax \cdot S1 \cdot S2 \cdot \left(1 - \frac{P1 \cdot P2}{Keq \cdot S1 \cdot S2}\right)}{Ks1 \cdot Ks2 \cdot \left(1 + \frac{S1}{Ks1} + \frac{P1}{Kp1}\right) \cdot \left(1 + \frac{S2}{Ks2} + \frac{P2}{Kp2} + \frac{I1}{Ki1} + \frac{I2}{Ki2}\right)} \tag{4}$$

5.5 Function definition mass_action_rev

Name mass_action_rev

Arguments k1, S, k2, P

Mathematical Expression

$$\mathrm{k1} \cdot \mathrm{S} - \mathrm{k2} \cdot \mathrm{P} \tag{5}$$

5.6 Function definition v1sub1prod

Name v1sub1prod

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

Mathematical Expression

$$\frac{\mathrm{Vfmax} \cdot \mathrm{S} \cdot \left(1 - \frac{\mathrm{P}}{\mathrm{Keq} \cdot \mathrm{S}}\right)}{\mathrm{Ks} \cdot \left(1 + \frac{\mathrm{S}}{\mathrm{Ks}} + \frac{\mathrm{P}}{\mathrm{Kp}}\right)} \tag{6}$$

5.7 Function definition mass_action_irrev

Name mass_action_irrev

Arguments k, S

Mathematical Expression

$$\mathrm{k} \cdot \mathrm{S} \tag{7}$$

6 Reactions

This model contains 36 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	TPI_g	TPI_g	$\mathrm{DHAP\_g} \xrightleftharpoons{\mathrm{DHAP\_g,\ GA3P\_g}} \mathrm{GA3P\_g}$	
2	PYK_c	PYK_c	$\mathrm{PEP\_c} + \mathrm{ADP\_c} \xrightleftharpoons{\mathrm{ADP\_c,\ Pyr\_c,\ ATP\_c,\ PEP\_c}} \mathrm{Pyr\_c} + \mathrm{ATP\_c}$	
3	PFK_g	PFK_g	$\mathrm{ATP\_g} + \mathrm{Fru6P\_g} \xrightleftharpoons{\mathrm{Fru6P\_g,\ ATP\_g,\ Fru16BP\_g,\ ADP\_g}} \mathrm{Fru16BP\_g} + \mathrm{ADP\_g}$	
4	G6PDH_g	G6PDH_g	$\mathrm{Glc6P\_g} + \mathrm{NADP\_g} \xrightleftharpoons{\mathrm{Glc6P\_g,\ NADP\_g,\ \_6PGL\_g,\ NADPH\_g}} \mathrm{\_6PGL\_g} + \mathrm{NADPH\_g}$	
5	PGAM_c	PGAM_c	$\mathrm{\_3PGA\_c} \xrightleftharpoons{\mathrm{\_3PGA\_c,\ \_2PGA\_c}} \mathrm{\_2PGA\_c}$	
6	PyrT_c	PyrT_c	$\mathrm{Pyr\_c} \xrightarrow{\mathrm{Pyr\_c}} \mathrm{Pyr\_e}$	
7	G6PDH_c	G6PDH_c	$\mathrm{Glc6P\_c} + \mathrm{NADP\_c} \xrightleftharpoons{\mathrm{Glc6P\_c,\ NADP\_c,\ \_6PGL\_c,\ NADPH\_c}} \mathrm{NADPH\_c} + \mathrm{\_6PGL\_c}$	
8	ENO_c	ENO_c	$\mathrm{\_2PGA\_c} \xrightleftharpoons{\mathrm{\_2PGA\_c,\ PEP\_c}} \mathrm{PEP\_c}$	
9	HXK_g	HXK_g	$\mathrm{ATP\_g} + \mathrm{Glc\_g} \xrightleftharpoons{\mathrm{Glc\_g,\ ATP\_g,\ Glc6P\_g,\ ADP\_g}} \mathrm{Glc6P\_g} + \mathrm{ADP\_g}$	
10	_3PGAT_g	_3PGAT_g	$\mathrm{\_3PGA\_g} \xrightleftharpoons{\mathrm{\_3PGA\_g,\ \_3PGA\_c}} \mathrm{\_3PGA\_c}$	
11	NADPHu_c	NADPHu_c	$\mathrm{NADPH\_c} \xrightarrow{\mathrm{NADPH\_c}} \mathrm{NADP\_c}$	

№	Id	Name	Reaction Equation	SBO
12	HXK_c	HXK_c	$\mathrm{Glc\_c} + \mathrm{ATP\_c} \xrightleftharpoons{\mathrm{Glc\_c,\ ATP\_c,\ Glc6P\_c,\ ADP\_c}} \mathrm{Glc6P\_c} + \mathrm{ADP\_c}$	
13	NADPHu_g	NADPHu_g	$\mathrm{NADPH\_g} \xrightarrow{\mathrm{NADPH\_g}} \mathrm{NADP\_g}$	
14	AK_c	AK_c	$2\,\mathrm{ADP\_c} \xrightleftharpoons{\mathrm{ADP\_c,\ AMP\_c,\ ATP\_c}} \mathrm{AMP\_c} + \mathrm{ATP\_c}$	
15	G6PP_c	G6PP_c	$\mathrm{Glc6P\_c} \xrightleftharpoons{\mathrm{Glc6P\_c,\ Glc\_c}} \mathrm{Glc\_c}$	
16	_6PGDH_g	_6PGDH_g	$\mathrm{\_6PG\_g} + \mathrm{NADP\_g} \xrightleftharpoons{\mathrm{\_6PG\_g,\ NADP\_g,\ Rul5P\_g,\ NADPH\_g}} \mathrm{Rul5P\_g} + \mathrm{CO2\_g} + \mathrm{NADPH\_g}$	
17	PGI_g	PGI_g	$\mathrm{Glc6P\_g} \xrightleftharpoons{\mathrm{\_6PG\_g,\ Glc6P\_g,\ Fru6P\_g,\ \_6PG\_g}} \mathrm{Fru6P\_g}$	
18	AK_g	AK_g	$2\,\mathrm{ADP\_g} \xrightleftharpoons{\mathrm{ADP\_g,\ AMP\_g,\ ATP\_g}} \mathrm{AMP\_g} + \mathrm{ATP\_g}$	
19	TOX_c	TOX_c	$\mathrm{TSH2\_c} \xrightarrow{\mathrm{TSH2\_c}} \mathrm{TS2\_c}$	
20	GDA_g	GDA_g	$\mathrm{Gly3P\_g} + \mathrm{DHAP\_c} \xrightleftharpoons{\mathrm{Gly3P\_g,\ DHAP\_c,\ Gly3P\_c,\ DHAP\_g}} \mathrm{Gly3P\_c} + \mathrm{DHAP\_g}$	
21	ATPT_g	ATPT_g	$\mathrm{ADP\_g} + \mathrm{ATP\_c} \xrightleftharpoons{\mathrm{ADP\_g,\ ATP\_c,\ ADP\_c,\ ATP\_g}} \mathrm{ATP\_g} + \mathrm{ADP\_c}$	
22	PGL_c	PGL_c	$\mathrm{\_6PGL\_c} \xrightleftharpoons{\mathrm{\_6PGL\_c,\ \_6PG\_c}} \mathrm{\_6PG\_c}$	
23	_6PGDH_c	_6PGDH_c	$\mathrm{NADP\_c} + \mathrm{\_6PG\_c} \xrightleftharpoons{\mathrm{\_6PG\_c,\ NADP\_c,\ Rul5P\_c,\ NADPH\_c}} \mathrm{CO2\_c} + \mathrm{NADPH\_c} + \mathrm{Rul5P\_c}$	
24	PPI_c	PPI_c	$\mathrm{Rul5P\_c} \xrightleftharpoons{\mathrm{Rul5P\_c,\ Rib5P\_c}} \mathrm{Rib5P\_c}$	
25	PPI_g	PPI_g	$\mathrm{Rul5P\_g} \xrightleftharpoons{\mathrm{Rul5P\_g,\ Rib5P\_g}} \mathrm{Rib5P\_g}$	
26	GlcT_g	GlcT_g	$\mathrm{Glc\_c} \xrightleftharpoons{\mathrm{Glc\_c,\ Glc\_g}} \mathrm{Glc\_g}$	
27	GlcT_c	GlcT_c	$\mathrm{Glc\_e} \xrightleftharpoons{\mathrm{Glc\_e,\ Glc\_c}} \mathrm{Glc\_c}$	

№	Id	Name	Reaction Equation	SBO
28	PGL_g	PGL_g	_6PGL_g $\xrightleftharpoons{\text{\_6PGL\_g, \_6PG\_g}}$ _6PG_g	
29	TR_c	TR_c	TS2_c + NADPH_c $\xrightleftharpoons{\text{TS2\_c, NADPH\_c, TSH2\_c, NADP\_c}}$ NADP_c + TSH2_c	
30	PGK_g	PGK_g	_13BPGA_g + ADP_g $\xrightleftharpoons{\text{\_13BPGA\_g, ADP\_g, \_3PGA\_g, ATP\_g}}$ _3PGA_g + ATP_g	
31	G3PDH_g	G3PDH_g	NADH_g + DHAP_g $\xrightleftharpoons{\text{DHAP\_g, NADH\_g, Gly3P\_g, NAD\_g}}$ Gly3P_g + NAD_g	
32	ATPu_c	ATPu_c	ATP_c $\xrightarrow{\text{ATP\_c, ADP\_c}}$ ADP_c	
33	GK_g	GK_g	Gly3P_g + ADP_g $\xrightleftharpoons{\text{Gly3P\_g, ADP\_g, Gly\_e, ATP\_g}}$ Gly_e + ATP_g	
34	ALD_g	ALD_g	Fru16BP_g $\xrightleftharpoons{\text{ATP\_g, ADP\_g, AMP\_g, Fru16BP\_g, GA3P\_g, DHAP\_g, ATP\_g, ADP\_g, A}}$ DHAP_g	
35	GAPDH_g	GAPDH_g	GA3P_g + NAD_g + Pi_g $\xrightleftharpoons{\text{GA3P\_g, NAD\_g, \_13BPGA\_g, NADH\_g}}$ NADH_g + _13BPGA_g	
36	GPO_c	GPO_c	Gly3P_c $\xrightarrow{\text{Gly3P\_c}}$ DHAP_c	

6.1 Reaction TPI_g

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

Name TPI_g

Reaction equation

$$\mathrm{DHAP\_g} \xrightleftharpoons{\mathrm{DHAP\_g,\ GA3P\_g}} \mathrm{GA3P\_g} \tag{8}$$

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	

Product

Table 7: Properties of each product.

Id	Name	SBO
GA3P_g	GA3P_g	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \mathrm{v1sub1prod}\left(\mathrm{TPI\_g\_Vmax}, \mathrm{TPI\_g\_Keq}, [\mathrm{DHAP\_g}], \mathrm{TPI\_g\_KmDHAP}, [\mathrm{GA3P\_g}], \mathrm{TPI\_g\_KmGA3P}\right) \tag{9}$$

$$\mathrm{v1sub1prod}\left(\mathrm{Vfmax}, \mathrm{Keq}, \mathrm{S}, \mathrm{Ks}, \mathrm{P}, \mathrm{Kp}\right) = \frac{\mathrm{Vfmax} \cdot \mathrm{S} \cdot \left(1 - \frac{\mathrm{P}}{\mathrm{Keq} \cdot \mathrm{S}}\right)}{\mathrm{Ks} \cdot \left(1 + \frac{\mathrm{S}}{\mathrm{Ks}} + \frac{\mathrm{P}}{\mathrm{Kp}}\right)} \tag{10}$$

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 four modifiers.

Name PYK_c

Reaction equation

$$\mathrm{PEP\_c} + \mathrm{ADP\_c} \xrightleftharpoons{\mathrm{ADP\_c,\ Pyr\_c,\ ATP\_c,\ PEP\_c}} \mathrm{Pyr\_c} + \mathrm{ATP\_c} \tag{11}$$

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	

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

$$v_2 = \frac{\text{PYK\_c\_Vmax} \cdot [\text{ADP\_c}] \cdot \left(1 - \frac{[\text{Pyr\_c}] \cdot [\text{ATP\_c}]}{\text{PYK\_c\_Keq} \cdot [\text{PEP\_c}] \cdot [\text{ADP\_c}]}\right) \cdot \left(\frac{[\text{PEP\_c}]}{\text{PYK\_c\_KmPEP} \cdot \left(1 + \frac{[\text{ADP\_c}]}{\text{PYK\_c\_KiADP}} + \frac{[\text{ATP\_c}]}{\text{PYK\_c\_KiATP}}\right)}\right)^{\text{PYK\_c}}}{\text{PYK\_c\_KmADP} \cdot \left(1 + \left(\frac{[\text{PEP\_c}]}{\text{PYK\_c\_KmPEP} \cdot \left(1 + \frac{[\text{ADP\_c}]}{\text{PYK\_c\_KiADP}} + \frac{[\text{ATP\_c}]}{\text{PYK\_c\_KiATP}}\right)}\right)^{\text{PYK\_c\_n}} + \frac{[\text{Pyr\_c}]}{\text{PYK\_c\_KmPyr}}\right) \cdot \left(1 + \frac{[\text{ADP\_c}]}{\text{PYK\_c\_KmADP}} + \text{P}\right.} \quad (12)$$

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 four modifiers.

Name PFK_g

Reaction equation

$$\text{ATP\_g} + \text{Fru6P\_g} \xrightleftharpoons{\text{Fru6P\_g, ATP\_g, Fru16BP\_g, ADP\_g}} \text{Fru16BP\_g} + \text{ADP\_g} \quad (13)$$

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	

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

$$v_3 = \frac{\text{PFK\_g\_Vmax} \cdot \text{PFK\_g\_Ki1} \cdot [\text{Fru6P\_g}] \cdot [\text{ATP\_g}] \cdot \left(1 - \frac{[\text{Fru}}{\text{PFK\_g\_K}}\right.}{\text{PFK\_g\_KmFru6P} \cdot \text{PFK\_g\_KmATP} \cdot ([\text{Fru16BP\_g}] + \text{PFK\_g\_Ki1}) \cdot \left(\frac{\text{PFK\_g\_KsATP}}{\text{PFK\_g\_KmATP}} + \frac{[\text{Fru6P\_g}]}{\text{PFK\_g\_KmFru6P}} + \frac{[\text{ATP\_g}]}{\text{PFK\_g\_KmATP}}\right.} \quad (14)$$

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		☑

Id	Name	SBO	Value	Unit	Constant
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 G6PDH_g

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

Name G6PDH_g

Reaction equation

$$\text{Glc6P\_g} + \text{NADP\_g} \xrightleftharpoons{\text{Glc6P\_g, NADP\_g, \_6PGL\_g, NADPH\_g}} \text{\_6PGL\_g} + \text{NADPH\_g} \quad (15)$$

Reactants

Table 17: Properties of each reactant.

Id	Name	SBO
Glc6P_g	Glc6P_g	
NADP_g	NADP_g	

Modifiers

Table 18: Properties of each modifier.

Id	Name	SBO
Glc6P_g	Glc6P_g	
NADP_g	NADP_g	
_6PGL_g	_6PGL_g	
NADPH_g	NADPH_g	

Products

Table 19: Properties of each product.

Id	Name	SBO
_6PGL_g	_6PGL_g	

Id	Name	SBO
NADPH_g	NADPH_g	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \text{v2sub2prod}\,(\text{G6PDH\_g\_Vmax}, \text{G6PDH\_g\_Keq}, [\text{Glc6P\_g}], \text{G6PDH\_g\_KmGlc6P}, [\text{NADP\_g}], \text{G6PDH\_g\_KmNADP}, [\text{\_6PGL\_g}], \text{G6PDH\_g\_Km6PGL}, [\text{NADPH\_g}], \text{G6PDH\_g\_KmNADPH}) \tag{16}$$

$$\text{v2sub2prod}\,(\text{Vfmax}, \text{Keq}, \text{S1}, \text{Ks1}, \text{S2}, \text{Ks2}, \text{P1}, \text{Kp1}, \text{P2}, \text{Kp2}) = \frac{\text{Vfmax} \cdot \text{S1} \cdot \text{S2} \cdot \left(1 - \frac{\text{P1} \cdot \text{P2}}{\text{Keq} \cdot \text{S1} \cdot \text{S2}}\right)}{\text{Ks1} \cdot \text{Ks2} \cdot \left(1 + \frac{\text{S1}}{\text{Ks1}} + \frac{\text{P1}}{\text{Kp1}}\right) \cdot \left(1 + \frac{\text{S2}}{\text{Ks2}} + \frac{\text{P2}}{\text{Kp2}}\right)} \tag{17}$$

Table 20: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
G6PDH_g_Vmax	G6PDH_g_Vmax		8.400		☑
G6PDH_g_Keq	G6PDH_g_Keq		5.020		☑
G6PDH_g_KmGlc6P	G6PDH_g_KmGlc6P		0.058		☑
G6PDH_g_KmNADP	G6PDH_g_KmNADP		0.009		☑
G6PDH_g_Km6PGL	G6PDH_g_Km6PGL		0.040		☑
G6PDH_g_KmNADPH	G6PDH_g_KmNADPH		10^{-4}		☑

6.5 Reaction PGAM_c

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

Name PGAM_c

Reaction equation

$$\text{\_3PGA\_c} \overset{\text{\_3PGA\_c, \_2PGA\_c}}{\rightleftharpoons} \text{\_2PGA\_c} \tag{18}$$

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	

Product

Table 23: Properties of each product.

Id	Name	SBO
_2PGA_c	_2PGA_c	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \text{v1sub1prod}\left(\text{PGAM\_c\_Vmax}, \text{PGAM\_c\_Keq}, [\text{\_3PGA\_c}], \text{PGAM\_c\_Km3PGA}, [\text{\_2PGA\_c}], \text{PGAM\_c\_Km2PGA}\right) \tag{19}$$

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

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		☑

6.6 Reaction PyrT_c

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

Name PyrT_c

Reaction equation

$$\text{Pyr\_c} \xrightarrow{\text{Pyr\_c}} \text{Pyr\_e} \tag{21}$$

Reactant

Table 25: Properties of each reactant.

Id	Name	SBO
Pyr_c	Pyr_c	

Modifier

Table 26: Properties of each modifier.

Id	Name	SBO
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

$$v_6 = \text{v1sub}\left(\text{PyrT\_c\_Vmax}, [\text{Pyr\_c}], \text{PyrT\_c\_KmPyr}\right) \tag{22}$$

$$\mathrm{v1sub}\left(\mathrm{Vfmax}, \mathrm{S}, \mathrm{Ks}\right) = \frac{\mathrm{Vfmax} \cdot \mathrm{S}}{\mathrm{Ks} \cdot \left(1 + \frac{\mathrm{S}}{\mathrm{Ks}}\right)} \tag{23}$$

Table 28: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
PyrT_c_Vmax	PyrT_c_Vmax		230.00		☑
PyrT_c_KmPyr	PyrT_c_KmPyr		1.96		☑

6.7 Reaction G6PDH_c

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

Name G6PDH_c

Reaction equation

$$\mathrm{Glc6P\_c} + \mathrm{NADP\_c} \xrightleftharpoons{\mathrm{Glc6P\_c,\ NADP\_c,\ \_6PGL\_c,\ NADPH\_c}} \mathrm{NADPH\_c} + \mathrm{\_6PGL\_c} \tag{24}$$

Reactants

Table 29: Properties of each reactant.

Id	Name	SBO
Glc6P_c	Glc6P_c	
NADP_c	NADP_c	

Modifiers

Table 30: Properties of each modifier.

Id	Name	SBO
Glc6P_c	Glc6P_c	
NADP_c	NADP_c	
_6PGL_c	_6PGL_c	
NADPH_c	NADPH_c	

Products

Table 31: Properties of each product.

Id	Name	SBO
NADPH_c	NADPH_c	
_6PGL_c	_6PGL_c	

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \text{v2sub2prod}\,(\text{G6PDH\_c\_Vmax}, \text{G6PDH\_c\_Keq}, [\text{Glc6P\_c}], \text{G6PDH\_c\_KmGlc6P}, [\text{NADP\_c}], \text{G6PDH\_c\_KmNADP}, [\text{\_6PGL\_c}], \text{G6PDH\_c\_Km6PGL}, [\text{NADPH\_c}], \text{G6PDH\_c\_KmNADPH}) \tag{25}$$

$$\text{v2sub2prod}\,(\text{Vfmax}, \text{Keq}, \text{S1}, \text{Ks1}, \text{S2}, \text{Ks2}, \text{P1}, \text{Kp1}, \text{P2}, \text{Kp2}) = \frac{\text{Vfmax} \cdot \text{S1} \cdot \text{S2} \cdot \left(1 - \frac{\text{P1} \cdot \text{P2}}{\text{Keq} \cdot \text{S1} \cdot \text{S2}}\right)}{\text{Ks1} \cdot \text{Ks2} \cdot \left(1 + \frac{\text{S1}}{\text{Ks1}} + \frac{\text{P1}}{\text{Kp1}}\right) \cdot \left(1 + \frac{\text{S2}}{\text{Ks2}} + \frac{\text{P2}}{\text{Kp2}}\right)} \tag{26}$$

Table 32: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
G6PDH_c_Vmax	G6PDH_c_Vmax		8.400		☑
G6PDH_c_Keq	G6PDH_c_Keq		5.020		☑
G6PDH_c_KmGlc6P	G6PDH_c_KmGlc6P		0.058		☑
G6PDH_c_KmNADP	G6PDH_c_KmNADP		0.009		☑
G6PDH_c_Km6PGL	G6PDH_c_Km6PGL		0.040		☑
G6PDH_c_KmNADPH	G6PDH_c_KmNADPH		10^{-4}		☑

6.8 Reaction ENO_c

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

Name ENO_c

Reaction equation

$$\_2PGA\_c \xrightleftharpoons{\_2PGA\_c,\ PEP\_c} PEP\_c \tag{27}$$

Reactant

Table 33: Properties of each reactant.

Id	Name	SBO
_2PGA_c	_2PGA_c	

Modifiers

Table 34: Properties of each modifier.

Id	Name	SBO
_2PGA_c	_2PGA_c	
PEP_c	PEP_c	

Product

Table 35: Properties of each product.

Id	Name	SBO
PEP_c	PEP_c	

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \mathrm{v1sub1prod}\left(\mathrm{ENO\_c\_Vmax}, \mathrm{ENO\_c\_Keq}, [\_2PGA\_c], \mathrm{ENO\_c\_Km2PGA}, [PEP\_c], \mathrm{ENO\_c\_KmPEP}\right) \tag{28}$$

$$\mathrm{v1sub1prod}\left(\mathrm{Vfmax}, \mathrm{Keq}, \mathrm{S}, \mathrm{Ks}, \mathrm{P}, \mathrm{Kp}\right) = \frac{\mathrm{Vfmax} \cdot \mathrm{S} \cdot \left(1 - \frac{\mathrm{P}}{\mathrm{Keq} \cdot \mathrm{S}}\right)}{\mathrm{Ks} \cdot \left(1 + \frac{\mathrm{S}}{\mathrm{Ks}} + \frac{\mathrm{P}}{\mathrm{Kp}}\right)} \tag{29}$$

Table 36: 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		☑

6.9 Reaction HXK_g

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

Name HXK_g

Reaction equation

$$\mathrm{ATP\_g} + \mathrm{Glc\_g} \xrightleftharpoons{\mathrm{Glc\_g,\ ATP\_g,\ Glc6P\_g,\ ADP\_g}} \mathrm{Glc6P\_g} + \mathrm{ADP\_g} \tag{30}$$

Reactants

Table 37: Properties of each reactant.

Id	Name	SBO
ATP_g	ATP_g	
Glc_g	Glc_g	

Modifiers

Table 38: Properties of each modifier.

Id	Name	SBO
Glc_g	Glc_g	
ATP_g	ATP_g	
Glc6P_g	Glc6P_g	
ADP_g	ADP_g	

Products

Table 39: Properties of each product.

Id	Name	SBO
Glc6P_g	Glc6P_g	
ADP_g	ADP_g	

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \text{v2sub2prod}\,(\text{HXK\_g\_Vmax}, \text{HXK\_g\_Keq}, [\text{Glc\_g}], \text{HXK\_g\_KmGlc}, [\text{ATP\_g}], \\ \text{HXK\_g\_KmATP}, [\text{Glc6P\_g}], \text{HXK\_g\_KmGlc6P}, [\text{ADP\_g}], \text{HXK\_g\_KmADP}) \tag{31}$$

$$\text{v2sub2prod}\,(\text{Vfmax}, \text{Keq}, \text{S1}, \text{Ks1}, \text{S2}, \text{Ks2}, \text{P1}, \text{Kp1}, \text{P2}, \text{Kp2}) \\ = \frac{\text{Vfmax} \cdot \text{S1} \cdot \text{S2} \cdot \left(1 - \frac{\text{P1} \cdot \text{P2}}{\text{Keq} \cdot \text{S1} \cdot \text{S2}}\right)}{\text{Ks1} \cdot \text{Ks2} \cdot \left(1 + \frac{\text{S1}}{\text{Ks1}} + \frac{\text{P1}}{\text{Kp1}}\right) \cdot \left(1 + \frac{\text{S2}}{\text{Ks2}} + \frac{\text{P2}}{\text{Kp2}}\right)} \tag{32}$$

Table 40: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
HXK_g_Vmax	HXK_g_Vmax		1774.680		☑
HXK_g_Keq	HXK_g_Keq		759.000		☑
HXK_g_KmGlc	HXK_g_KmGlc		0.100		☑
HXK_g_KmATP	HXK_g_KmATP		0.116		☑
HXK_g_KmGlc6P	HXK_g_KmGlc6P		2.700		☑
HXK_g_KmADP	HXK_g_KmADP		0.126		☑

6.10 Reaction _3PGAT_g

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

Name _3PGAT_g

Reaction equation

$$\text{\_3PGA\_g} \underset{\text{\_3PGA\_g, \_3PGA\_c}}{\rightleftharpoons} \text{\_3PGA\_c} \tag{33}$$

Reactant

Table 41: Properties of each reactant.

Id	Name	SBO
_3PGA_g	_3PGA_g	

Modifiers

Table 42: Properties of each modifier.

Id	Name	SBO
_3PGA_g	_3PGA_g	
_3PGA_c	_3PGA_c	

Product

Table 43: Properties of each product.

Id	Name	SBO
_3PGA_c	_3PGA_c	

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = \text{mass\_action\_rev}\left(\text{\_3PGAT\_g\_k}, [\text{\_3PGA\_g}], \text{\_3PGAT\_g\_k}, [\text{\_3PGA\_c}]\right) \tag{34}$$

$$\text{mass\_action\_rev}\left(\text{k1}, \text{S}, \text{k2}, \text{P}\right) = \text{k1} \cdot \text{S} - \text{k2} \cdot \text{P} \tag{35}$$

Table 44: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
_3PGAT_g_k	_3PGAT_g_k		250.0		☑

6.11 Reaction NADPHu_c

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

Name NADPHu_c

Reaction equation

$$\text{NADPH\_c} \xrightarrow{\text{NADPH\_c}} \text{NADP\_c} \tag{36}$$

Reactant

Table 45: Properties of each reactant.

Id	Name	SBO
NADPH_c	NADPH_c	

Modifier

Table 46: Properties of each modifier.

Id	Name	SBO
NADPH_c	NADPH_c	

Product

Table 47: Properties of each product.

Id	Name	SBO
NADP_c	NADP_c	

Kinetic Law

Derived unit contains undeclared units

$$v_{11} = \text{mass\_action\_irrev}\left(\text{NADPHu\_c\_k}, [\text{NADPH\_c}]\right) \tag{37}$$

$$\text{mass\_action\_irrev}\left(\text{k}, \text{S}\right) = \text{k} \cdot \text{S} \tag{38}$$

Table 48: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
NADPHu_c_k	NADPHu_c_k		2.0		☑

6.12 Reaction HXK_c

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

Name HXK_c

Reaction equation

$$\text{Glc\_c} + \text{ATP\_c} \xrightleftharpoons{\text{Glc\_c, ATP\_c, Glc6P\_c, ADP\_c}} \text{Glc6P\_c} + \text{ADP\_c} \tag{39}$$

Reactants

Table 49: Properties of each reactant.

Id	Name	SBO
Glc_c	Glc_c	
ATP_c	ATP_c	

Modifiers

Table 50: Properties of each modifier.

Id	Name	SBO
Glc_c	Glc_c	
ATP_c	ATP_c	
Glc6P_c	Glc6P_c	
ADP_c	ADP_c	

Products

Table 51: Properties of each product.

Id	Name	SBO
Glc6P_c	Glc6P_c	
ADP_c	ADP_c	

Kinetic Law

Derived unit contains undeclared units

$$\begin{aligned} v_{12} = \text{v2sub2prod}\,(&\text{HXK\_c\_Vmax}, \text{HXK\_c\_Keq}, [\text{Glc\_c}], \text{HXK\_c\_KmGlc}, [\text{ATP\_c}], \\ &\text{HXK\_c\_KmATP}, [\text{Glc6P\_c}], \text{HXK\_c\_KmGlc6P}, [\text{ADP\_c}], \text{HXK\_c\_KmADP}) \end{aligned} \tag{40}$$

$$\begin{aligned}&\text{v2sub2prod}\left(\text{Vfmax}, \text{Keq}, \text{S1}, \text{Ks1}, \text{S2}, \text{Ks2}, \text{P1}, \text{Kp1}, \text{P2}, \text{Kp2}\right)\\&= \frac{\text{Vfmax} \cdot \text{S1} \cdot \text{S2} \cdot \left(1 - \frac{\text{P1} \cdot \text{P2}}{\text{Keq} \cdot \text{S1} \cdot \text{S2}}\right)}{\text{Ks1} \cdot \text{Ks2} \cdot \left(1 + \frac{\text{S1}}{\text{Ks1}} + \frac{\text{P1}}{\text{Kp1}}\right) \cdot \left(1 + \frac{\text{S2}}{\text{Ks2}} + \frac{\text{P2}}{\text{Kp2}}\right)}\end{aligned} \tag{41}$$

Table 52: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
HXK_c_Vmax	HXK_c_Vmax		154.320		☑
HXK_c_Keq	HXK_c_Keq		759.000		☑
HXK_c_KmGlc	HXK_c_KmGlc		0.100		☑
HXK_c_KmATP	HXK_c_KmATP		0.116		☑
HXK_c_KmGlc6P	HXK_c_KmGlc6P		2.700		☑
HXK_c_KmADP	HXK_c_KmADP		0.126		☑

6.13 Reaction NADPHu_g

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

Name NADPHu_g

Reaction equation

$$\text{NADPH\_g} \xrightarrow{\text{NADPH\_g}} \text{NADP\_g} \tag{42}$$

Reactant

Table 53: Properties of each reactant.

Id	Name	SBO
NADPH_g	NADPH_g	

Modifier

Table 54: Properties of each modifier.

Id	Name	SBO
NADPH_g	NADPH_g	

Product

Table 55: Properties of each product.

Id	Name	SBO
NADP_g	NADP_g	

Kinetic Law

Derived unit contains undeclared units

$$v_{13} = \text{mass\_action\_irrev}\left(\text{NADPHu\_g\_k}, [\text{NADPH\_g}]\right) \tag{43}$$

$$\text{mass\_action\_irrev}\left(\text{k}, \text{S}\right) = \text{k} \cdot \text{S} \tag{44}$$

Table 56: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
NADPHu_g_k	NADPHu_g_k		2.0		☑

6.14 Reaction AK_c

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

Name AK_c

Reaction equation

$$2\,\text{ADP\_c} \xrightleftharpoons{\text{ADP\_c, AMP\_c, ATP\_c}} \text{AMP\_c} + \text{ATP\_c} \tag{45}$$

Reactant

Table 57: Properties of each reactant.

Id	Name	SBO
ADP_c	ADP_c	

Modifiers

Table 58: Properties of each modifier.

Id	Name	SBO
ADP_c	ADP_c	
AMP_c	AMP_c	
ATP_c	ATP_c	

Products

Table 59: Properties of each product.

Id	Name	SBO
AMP_c	AMP_c	
ATP_c	ATP_c	

Kinetic Law

Derived unit contains undeclared units

$$v_{14} = \mathrm{vAK}\left([\mathrm{ADP\_c}], [\mathrm{AMP\_c}], [\mathrm{ATP\_c}], \mathrm{AK\_c\_k1}, \mathrm{AK\_c\_k2}\right) \tag{46}$$

$$\mathrm{vAK}\left(\mathrm{ADP}, \mathrm{AMP}, \mathrm{ATP}, \mathrm{k1}, \mathrm{k2}\right) = \mathrm{k1} \cdot \mathrm{ADP}^2 - \mathrm{AMP} \cdot \mathrm{ATP} \cdot \mathrm{k2} \tag{47}$$

Table 60: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
AK_c_k1	AK_c_k1		480.0		☑
AK_c_k2	AK_c_k2		1000.0		☑

6.15 Reaction G6PP_c

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

Name G6PP_c

Reaction equation

$$\mathrm{Glc6P\_c} \xrightleftharpoons{\mathrm{Glc6P\_c},\ \mathrm{Glc\_c}} \mathrm{Glc\_c} \tag{48}$$

Reactant

Table 61: Properties of each reactant.

Id	Name	SBO
Glc6P_c	Glc6P_c	

Modifiers

Table 62: Properties of each modifier.

Id	Name	SBO
Glc6P_c	Glc6P_c	
Glc_c	Glc_c	

Product

Table 63: Properties of each product.

Id	Name	SBO
Glc_c	Glc_c	

Kinetic Law

Derived unit contains undeclared units

$$v_{15} = \mathrm{v1sub1prod}\left(\mathrm{G6PP\_c\_Vmax}, \mathrm{G6PP\_c\_Keq}, [\mathrm{Glc6P\_c}], \mathrm{G6PP\_c\_KmGlc6P}, [\mathrm{Glc\_c}], \mathrm{G6PP\_c\_KmGlc}\right) \tag{49}$$

$$\mathrm{v1sub1prod}\left(\mathrm{Vfmax}, \mathrm{Keq}, \mathrm{S}, \mathrm{Ks}, \mathrm{P}, \mathrm{Kp}\right) = \frac{\mathrm{Vfmax} \cdot \mathrm{S} \cdot \left(1 - \frac{\mathrm{P}}{\mathrm{Keq} \cdot \mathrm{S}}\right)}{\mathrm{Ks} \cdot \left(1 + \frac{\mathrm{S}}{\mathrm{Ks}} + \frac{\mathrm{P}}{\mathrm{Kp}}\right)} \tag{50}$$

Table 64: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
G6PP_c_Vmax	G6PP_c_Vmax		28.0		☑
G6PP_c_Keq	G6PP_c_Keq		263.0		☑
G6PP_c-_KmGlc6P	G6PP_c_KmGlc6P		5.6		☑
G6PP_c_KmGlc	G6PP_c_KmGlc		5.6		☑

6.16 Reaction _6PGDH_g

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

Name _6PGDH_g

Reaction equation

$$\text{\_6PG\_g} + \text{NADP\_g} \xrightleftharpoons{\text{\_6PG\_g, NADP\_g, Rul5P\_g, NADPH\_g}} \text{Rul5P\_g} + \text{CO2\_g} + \text{NADPH\_g} \tag{51}$$

Reactants

Table 65: Properties of each reactant.

Id	Name	SBO
_6PG_g	_6PG_g	
NADP_g	NADP_g	

Modifiers

Table 66: Properties of each modifier.

Id	Name	SBO
_6PG_g	_6PG_g	
NADP_g	NADP_g	
Rul5P_g	Rul5P_g	
NADPH_g	NADPH_g	

Products

Table 67: Properties of each product.

Id	Name	SBO
Rul5P_g	Rul5P_g	
CO2_g	CO2_g	
NADPH_g	NADPH_g	

Kinetic Law

Derived unit contains undeclared units

$$v_{16} = \text{v2sub2prod}\,(\text{\_6PGDH\_g\_Vmax}, \text{\_6PGDH\_g\_Keq}, [\text{\_6PG\_g}], \text{\_6PGDH\_g\_Km6PG}, [\text{NADP\_g}], \text{\_6PGDH\_g\_KmNADP}, [\text{Rul5P\_g}], \text{\_6PGDH\_g\_KmRul5P}, [\text{NADPH\_g}], \text{\_6PGDH\_g\_KmNADPH}) \tag{52}$$

$$\text{v2sub2prod}\,(\text{Vfmax}, \text{Keq}, \text{S1}, \text{Ks1}, \text{S2}, \text{Ks2}, \text{P1}, \text{Kp1}, \text{P2}, \text{Kp2}) = \frac{\text{Vfmax} \cdot \text{S1} \cdot \text{S2} \cdot \left(1 - \frac{\text{P1} \cdot \text{P2}}{\text{Keq} \cdot \text{S1} \cdot \text{S2}}\right)}{\text{Ks1} \cdot \text{Ks2} \cdot \left(1 + \frac{\text{S1}}{\text{Ks1}} + \frac{\text{P1}}{\text{Kp1}}\right) \cdot \left(1 + \frac{\text{S2}}{\text{Ks2}} + \frac{\text{P2}}{\text{Kp2}}\right)} \tag{53}$$

Table 68: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
_6PGDH_g_Vmax	_6PGDH_g_Vmax		10.600		☑
_6PGDH_g_Keq	_6PGDH_g_Keq		47.000		☑
_6PGDH_g_Km6PG	_6PGDH_g_Km6PG		0.004		☑
_6PGDH_g_KmNADP	_6PGDH_g_KmNADP		0.001		☑
_6PGDH_g_KmRul5P	_6PGDH_g_KmRul5P		0.030		☑
_6PGDH_g_KmNADPH	_6PGDH_g_KmNADPH		$6 \cdot 10^{-4}$		☑

6.17 Reaction PGI_g

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

Name PGI_g

Reaction equation

$$\text{Glc6P\_g} \xrightleftharpoons{\text{\_6PG\_g, Glc6P\_g, Fru6P\_g, \_6PG\_g}} \text{Fru6P\_g} \tag{54}$$

Reactant

Table 69: Properties of each reactant.

Id	Name	SBO
Glc6P_g	Glc6P_g	

Modifiers

Table 70: Properties of each modifier.

Id	Name	SBO
_6PG_g	_6PG_g	
Glc6P_g	Glc6P_g	
Fru6P_g	Fru6P_g	
_6PG_g	_6PG_g	

Product

Table 71: Properties of each product.

Id	Name	SBO
Fru6P_g	Fru6P_g	

Kinetic Law

Derived unit contains undeclared units

$$v_{17} = \frac{\text{PGI\_g\_Vmax} \cdot [\text{Glc6P\_g}] \cdot \left(1 - \frac{[\text{Fru6P\_g}]}{\text{PGI\_g\_Keq} \cdot [\text{Glc6P\_g}]}\right)}{\text{PGI\_g\_KmGlc6P} \cdot \left(1 + \frac{[\text{Glc6P\_g}]}{\text{PGI\_g\_KmGlc6P}} + \frac{[\text{Fru6P\_g}]}{\text{PGI\_g\_KmFru6P}} + \frac{[\text{\_6PG\_g}]}{\text{PGI\_g\_Ki6PG}}\right)} \tag{55}$$

Table 72: 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		☑
PGI_g_Ki6PG	PGI_g_Ki6PG		0.140		☑

6.18 Reaction AK_g

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

Name AK_g

Reaction equation

$$2\,\mathrm{ADP\_g} \rightleftharpoons{\mathrm{ADP\_g,\ AMP\_g,\ ATP\_g}} \mathrm{AMP\_g} + \mathrm{ATP\_g} \tag{56}$$

Reactant

Table 73: Properties of each reactant.

Id	Name	SBO
ADP_g	ADP_g	

Modifiers

Table 74: Properties of each modifier.

Id	Name	SBO
ADP_g	ADP_g	
AMP_g	AMP_g	
ATP_g	ATP_g	

Products

Table 75: Properties of each product.

Id	Name	SBO
AMP_g	AMP_g	
ATP_g	ATP_g	

Kinetic Law

Derived unit contains undeclared units

$$v_{18} = \mathrm{vAK}\left([\mathrm{ADP\_g}], [\mathrm{AMP\_g}], [\mathrm{ATP\_g}], \mathrm{AK\_g\_k1}, \mathrm{AK\_g\_k2}\right) \tag{57}$$

$$\mathrm{vAK}\left(\mathrm{ADP}, \mathrm{AMP}, \mathrm{ATP}, \mathrm{k1}, \mathrm{k2}\right) = \mathrm{k1} \cdot \mathrm{ADP}^2 - \mathrm{AMP} \cdot \mathrm{ATP} \cdot \mathrm{k2} \tag{58}$$

Table 76: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
AK_g_k1	AK_g_k1		480.0		☑
AK_g_k2	AK_g_k2		1000.0		☑

6.19 Reaction TOX_c

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

Name TOX_c

Reaction equation

$$\mathrm{TSH2\_c} \xrightarrow{\mathrm{TSH2\_c}} \mathrm{TS2\_c} \tag{59}$$

Reactant

Table 77: Properties of each reactant.

Id	Name	SBO
TSH2_c	TSH2_c	

Modifier

Table 78: Properties of each modifier.

Id	Name	SBO
TSH2_c	TSH2_c	

Product

Table 79: Properties of each product.

Id	Name	SBO
TS2_c	TS2_c	

Kinetic Law

Derived unit contains undeclared units

$$v_{19} = \mathrm{mass\_action\_irrev}\left(\mathrm{TOX\_c\_k}, [\mathrm{TSH2\_c}]\right) \tag{60}$$

$$\mathrm{mass\_action\_irrev}\left(\mathrm{k}, \mathrm{S}\right) = \mathrm{k} \cdot \mathrm{S} \tag{61}$$

Table 80: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
TOX_c_k	TOX_c_k		2.0		☑

6.20 Reaction GDA_g

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

Name GDA_g

Reaction equation

$$\text{Gly3P\_g} + \text{DHAP\_c} \xrightleftharpoons{\text{Gly3P\_g, DHAP\_c, Gly3P\_c, DHAP\_g}} \text{Gly3P\_c} + \text{DHAP\_g} \qquad (62)$$

Reactants

Table 81: Properties of each reactant.

Id	Name	SBO
Gly3P_g	Gly3P_g	
DHAP_c	DHAP_c	

Modifiers

Table 82: Properties of each modifier.

Id	Name	SBO
Gly3P_g	Gly3P_g	
DHAP_c	DHAP_c	
Gly3P_c	Gly3P_c	
DHAP_g	DHAP_g	

Products

Table 83: Properties of each product.

Id	Name	SBO
Gly3P_c	Gly3P_c	
DHAP_g	DHAP_g	

Kinetic Law

Derived unit contains undeclared units

$$v_{20} = [\text{Gly3P\_g}] \cdot \text{GDA\_g\_k} \cdot [\text{DHAP\_c}] - [\text{Gly3P\_c}] \cdot \text{GDA\_g\_k} \cdot [\text{DHAP\_g}] \tag{63}$$

Table 84: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
GDA_g_k	GDA_g_k		600.0		☑

6.21 Reaction ATPT_g

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

Name ATPT_g

Reaction equation

$$\text{ADP\_g} + \text{ATP\_c} \xrightleftharpoons{\text{ADP\_g, ATP\_c, ADP\_c, ATP\_g}} \text{ATP\_g} + \text{ADP\_c} \tag{64}$$

Reactants

Table 85: Properties of each reactant.

Id	Name	SBO
ADP_g	ADP_g	
ATP_c	ATP_c	

Modifiers

Table 86: Properties of each modifier.

Id	Name	SBO
ADP_g	ADP_g	
ATP_c	ATP_c	
ADP_c	ADP_c	
ATP_g	ATP_g	

Products

Table 87: Properties of each product.

Id	Name	SBO
ATP_g	ATP_g	
ADP_c	ADP_c	

Kinetic Law

Derived unit contains undeclared units

$$v_{21} = \text{v2sub2prod}\left(\text{ATPT\_g\_Vmax}, \text{ATPT\_g\_Keq}, [\text{ADP\_g}], \text{ATPT\_g\_KmADP}, [\text{ATP\_c}], \text{ATPT\_g\_KmATP}, [\text{ADP\_c}], \text{ATPT\_g\_KmADP}, [\text{ATP\_g}], \text{ATPT\_g\_KmATP}\right) \tag{65}$$

$$\text{v2sub2prod}\left(\text{Vfmax}, \text{Keq}, \text{S1}, \text{Ks1}, \text{S2}, \text{Ks2}, \text{P1}, \text{Kp1}, \text{P2}, \text{Kp2}\right) = \frac{\text{Vfmax} \cdot \text{S1} \cdot \text{S2} \cdot \left(1 - \frac{\text{P1} \cdot \text{P2}}{\text{Keq} \cdot \text{S1} \cdot \text{S2}}\right)}{\text{Ks1} \cdot \text{Ks2} \cdot \left(1 + \frac{\text{S1}}{\text{Ks1}} + \frac{\text{P1}}{\text{Kp1}}\right) \cdot \left(1 + \frac{\text{S2}}{\text{Ks2}} + \frac{\text{P2}}{\text{Kp2}}\right)} \tag{66}$$

Table 88: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
ATPT_g_Vmax	ATPT_g_Vmax		1.50		☑
ATPT_g_Keq	ATPT_g_Keq		1.00		☑
ATPT_g_KmADP	ATPT_g_KmADP		0.02		☑
ATPT_g_KmATP	ATPT_g_KmATP		0.02		☑

6.22 Reaction PGL_c

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

Name PGL_c

Reaction equation

$$\text{\_6PGL\_c} \xrightleftharpoons{\text{\_6PGL\_c, \_6PG\_c}} \text{\_6PG\_c} \tag{67}$$

Reactant

Table 89: Properties of each reactant.

Id	Name	SBO
_6PGL_c	_6PGL_c	

Modifiers

Table 90: Properties of each modifier.

Id	Name	SBO
_6PGL_c	_6PGL_c	
_6PG_c	_6PG_c	

Product

Table 91: Properties of each product.

Id	Name	SBO
_6PG_c	_6PG_c	

Kinetic Law

Derived unit contains undeclared units

$$v_{22} = \mathrm{PGL\_c\_k} \cdot \mathrm{vol}\left(\mathrm{cytosol}\right) \cdot \left(\left[\mathrm{\_6PGL\_c}\right] - \frac{\left[\mathrm{\_6PG\_c}\right]}{\mathrm{PGL\_c\_Keq}} \right) + \mathrm{v1sub1prod}\left(\mathrm{PGL\_c\_Vmax}, \mathrm{PGL\_c\_Keq}, \left[\mathrm{\_6PGL\_c}\right], \mathrm{PGL\_c\_Km6PGL}, \left[\mathrm{\_6PG\_c}\right], \mathrm{PGL\_c\_Km6PG}\right) \tag{68}$$

$$\mathrm{v1sub1prod}\left(\mathrm{Vfmax}, \mathrm{Keq}, \mathrm{S}, \mathrm{Ks}, \mathrm{P}, \mathrm{Kp}\right) = \frac{\mathrm{Vfmax} \cdot \mathrm{S} \cdot \left(1 - \frac{\mathrm{P}}{\mathrm{Keq} \cdot \mathrm{S}}\right)}{\mathrm{Ks} \cdot \left(1 + \frac{\mathrm{S}}{\mathrm{Ks}} + \frac{\mathrm{P}}{\mathrm{Kp}}\right)} \tag{69}$$

$$\mathrm{v1sub1prod}\left(\mathrm{Vfmax}, \mathrm{Keq}, \mathrm{S}, \mathrm{Ks}, \mathrm{P}, \mathrm{Kp}\right) = \frac{\mathrm{Vfmax} \cdot \mathrm{S} \cdot \left(1 - \frac{\mathrm{P}}{\mathrm{Keq} \cdot \mathrm{S}}\right)}{\mathrm{Ks} \cdot \left(1 + \frac{\mathrm{S}}{\mathrm{Ks}} + \frac{\mathrm{P}}{\mathrm{Kp}}\right)} \tag{70}$$

Table 92: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
PGL_c_Vmax	PGL_c_Vmax		28.000		☑
PGL_c_Keq	PGL_c_Keq		20000.000		☑
PGL_c_Km6PGL	PGL_c_Km6PGL		0.050		☑
PGL_c_Km6PG	PGL_c_Km6PG		0.050		☑
PGL_c_k	PGL_c_k		0.055		☑

6.23 Reaction _6PGDH_c

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

Name _6PGDH_c

Reaction equation

$$\mathrm{NADP\_c} + \mathrm{\_6PG\_c} \xrightleftharpoons{\mathrm{\_6PG\_c,\ NADP\_c,\ Rul5P\_c,\ NADPH\_c}} \mathrm{CO2\_c} + \mathrm{NADPH\_c} + \mathrm{Rul5P\_c} \tag{71}$$

Reactants

Table 93: Properties of each reactant.

Id	Name	SBO
NADP_c	NADP_c	
_6PG_c	_6PG_c	

Modifiers

Table 94: Properties of each modifier.

Id	Name	SBO
_6PG_c	_6PG_c	
NADP_c	NADP_c	
Rul5P_c	Rul5P_c	
NADPH_c	NADPH_c	

Products

Table 95: Properties of each product.

Id	Name	SBO
CO2_c	CO2_c	
NADPH_c	NADPH_c	
Ru5P_c	Ru5P_c	

Kinetic Law

Derived unit contains undeclared units

$$v_{23} = \text{v2sub2prod}(\text{\_6PGDH\_c\_Vmax}, \text{\_6PGDH\_c\_Keq}, [\text{\_6PG\_c}], \text{\_6PGDH\_c\_Km6PG}, [\text{NADP\_c}], \text{\_6PGDH\_c\_KmNADP}, [\text{Ru5P\_c}], \text{\_6PGDH\_c\_KmRu5P}, [\text{NADPH\_c}], \text{\_6PGDH\_c\_KmNADPH}) \quad (72)$$

$$\text{v2sub2prod}(\text{Vfmax}, \text{Keq}, \text{S1}, \text{Ks1}, \text{S2}, \text{Ks2}, \text{P1}, \text{Kp1}, \text{P2}, \text{Kp2}) = \frac{\text{Vfmax} \cdot \text{S1} \cdot \text{S2} \cdot \left(1 - \frac{\text{P1} \cdot \text{P2}}{\text{Keq} \cdot \text{S1} \cdot \text{S2}}\right)}{\text{Ks1} \cdot \text{Ks2} \cdot \left(1 + \frac{\text{S1}}{\text{Ks1}} + \frac{\text{P1}}{\text{Kp1}}\right) \cdot \left(1 + \frac{\text{S2}}{\text{Ks2}} + \frac{\text{P2}}{\text{Kp2}}\right)} \quad (73)$$

Table 96: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
_6PGDH_c_Vmax	_6PGDH_c_Vmax		10.600		☑
_6PGDH_c_Keq	_6PGDH_c_Keq		47.000		☑
_6PGDH_c_Km6PG	_6PGDH_c_Km6PG		0.004		☑
_6PGDH_c_KmNADP	_6PGDH_c_KmNADP		0.001		☑
_6PGDH_c_KmRu5P	_6PGDH_c_KmRu5P		0.030		☑
_6PGDH_c_KmNADPH	_6PGDH_c_KmNADPH		$6 \cdot 10^{-4}$		☑

6.24 Reaction PPI_c

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

Name PPI_c

Reaction equation

$$\text{Rul5P\_c} \underset{\text{Rul5P\_c, Rib5P\_c}}{\rightleftharpoons} \text{Rib5P\_c} \tag{74}$$

Reactant

Table 97: Properties of each reactant.

Id	Name	SBO
Rul5P_c	Rul5P_c	

Modifiers

Table 98: Properties of each modifier.

Id	Name	SBO
Rul5P_c	Rul5P_c	
Rib5P_c	Rib5P_c	

Product

Table 99: Properties of each product.

Id	Name	SBO
Rib5P_c	Rib5P_c	

Kinetic Law

Derived unit contains undeclared units

$$v_{24} = \text{v1sub1prod}\left(\text{PPI\_c\_Vmax}, \text{PPI\_c\_Keq}, [\text{Rul5P\_c}], \text{PPI\_c\_KmRul5P}, [\text{Rib5P\_c}], \text{PPI\_c\_KmRib5P}\right) \tag{75}$$

$$\text{v1sub1prod}\left(\text{Vfmax}, \text{Keq}, \text{S}, \text{Ks}, \text{P}, \text{Kp}\right) = \frac{\text{Vfmax} \cdot \text{S} \cdot \left(1 - \frac{\text{P}}{\text{Keq} \cdot \text{S}}\right)}{\text{Ks} \cdot \left(1 + \frac{\text{S}}{\text{Ks}} + \frac{\text{P}}{\text{Kp}}\right)} \tag{76}$$

Table 100: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
PPI_c_Vmax	PPI_c_Vmax		72.0		☑
PPI_c_Keq	PPI_c_Keq		5.6		☑
PPI_c_KmRul5P	PPI_c_KmRul5P		1.4		☑
PPI_c_KmRib5P	PPI_c_KmRib5P		4.0		☑

6.25 Reaction PPI_g

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

Name PPI_g

Reaction equation

$$\mathrm{Rul5P\_g} \xrightleftharpoons{\mathrm{Rul5P\_g,\ Rib5P\_g}} \mathrm{Rib5P\_g} \tag{77}$$

Reactant

Table 101: Properties of each reactant.

Id	Name	SBO
Rul5P_g	Rul5P_g	

Modifiers

Table 102: Properties of each modifier.

Id	Name	SBO
Rul5P_g	Rul5P_g	
Rib5P_g	Rib5P_g	

Product

Table 103: Properties of each product.

Id	Name	SBO
Rib5P_g	Rib5P_g	

Kinetic Law

Derived unit contains undeclared units

$$v_{25} = \text{v1sub1prod}\left(\text{PPI\_g\_Vmax}, \text{PPI\_g\_Keq}, [\text{Rul5P\_g}], \text{PPI\_g\_KmRul5P}, [\text{Rib5P\_g}], \text{PPI\_g\_KmRib5P}\right) \tag{78}$$

$$\text{v1sub1prod}\left(\text{Vfmax}, \text{Keq}, \text{S}, \text{Ks}, \text{P}, \text{Kp}\right) = \frac{\text{Vfmax} \cdot \text{S} \cdot \left(1 - \frac{\text{P}}{\text{Keq} \cdot \text{S}}\right)}{\text{Ks} \cdot \left(1 + \frac{\text{S}}{\text{Ks}} + \frac{\text{P}}{\text{Kp}}\right)} \tag{79}$$

Table 104: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
PPI_g_Vmax	PPI_g_Vmax		72.0		☑
PPI_g_Keq	PPI_g_Keq		5.6		☑
PPI_g_KmRul5P	PPI_g_KmRul5P		1.4		☑
PPI_g_KmRib5P	PPI_g_KmRib5P		4.0		☑

6.26 Reaction GlcT_g

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

Name GlcT_g

Reaction equation

$$\text{Glc\_c} \xrightleftharpoons{\text{Glc\_c, Glc\_g}} \text{Glc\_g} \tag{80}$$

Reactant

Table 105: Properties of each reactant.

Id	Name	SBO
Glc_c	Glc_c	

Modifiers

Table 106: Properties of each modifier.

Id	Name	SBO
Glc_c	Glc_c	
Glc_g	Glc_g	

Product

Table 107: Properties of each product.

Id	Name	SBO
Glc_g	Glc_g	

Kinetic Law

Derived unit contains undeclared units

$$v_{26} = \text{mass\_action\_rev}\left(\text{GlcT\_g\_k1}, [\text{Glc\_c}], \text{GlcT\_g\_k2}, [\text{Glc\_g}]\right) \tag{81}$$

$$\text{mass\_action\_rev}\left(\text{k1}, \text{S}, \text{k2}, \text{P}\right) = \text{k1} \cdot \text{S} - \text{k2} \cdot \text{P} \tag{82}$$

Table 108: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
GlcT_g_k1	GlcT_g_k1		250000.0		☑
GlcT_g_k2	GlcT_g_k2		250000.0		☑

6.27 Reaction GlcT_c

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

Name GlcT_c

Reaction equation

$$\text{Glc\_e} \xrightleftharpoons{\text{Glc\_e, Glc\_c}} \text{Glc\_c} \tag{83}$$

Reactant

Table 109: Properties of each reactant.

Id	Name	SBO
Glc_e	Glc_e	

Modifiers

Table 110: Properties of each modifier.

Id	Name	SBO
Glc_e	Glc_e	
Glc_c	Glc_c	

Product

Table 111: Properties of each product.

Id	Name	SBO
Glc_c	Glc_c	

Kinetic Law

Derived unit contains undeclared units

$$v_{27} = \frac{\text{GlcT\_c\_Vmax} \cdot ([\text{Glc\_e}] - [\text{Glc\_c}])}{\text{GlcT\_c\_KmGlc} + [\text{Glc\_e}] + [\text{Glc\_c}] + \frac{\text{GlcT\_c\_alpha} \cdot [\text{Glc\_e}] \cdot [\text{Glc\_c}]}{\text{GlcT\_c\_KmGlc}}} \tag{84}$$

Table 112: 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		☑

6.28 Reaction PGL_g

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

Name PGL_g

Reaction equation

$$\_6PGL\_g \xrightleftharpoons{\_6PGL\_g,\ \_6PG\_g} \_6PG\_g \tag{85}$$

Reactant

Table 113: Properties of each reactant.

Id	Name	SBO
_6PGL_g	_6PGL_g	

Modifiers

Table 114: Properties of each modifier.

Id	Name	SBO
_6PGL_g	_6PGL_g	
_6PG_g	_6PG_g	

Product

Table 115: Properties of each product.

Id	Name	SBO
_6PG_g	_6PG_g	

Kinetic Law

Derived unit contains undeclared units

$$v_{28} = \mathrm{vol}(\mathrm{glycosome}) \cdot \mathrm{PGL\_g\_k} \cdot \left([\_6PGL\_g] - \frac{[\_6PG\_g]}{\mathrm{PGL\_g\_Keq}} \right) + \mathrm{v1sub1prod}(\mathrm{PGL\_g\_Vmax}, \mathrm{PGL\_g\_Keq}, [\_6PGL\_g], \mathrm{PGL\_g\_Km6PGL}, [\_6PG\_g], \mathrm{PGL\_g\_Km6PG}) \tag{86}$$

$$\mathrm{v1sub1prod}(\mathrm{Vfmax}, \mathrm{Keq}, \mathrm{S}, \mathrm{Ks}, \mathrm{P}, \mathrm{Kp}) = \frac{\mathrm{Vfmax} \cdot \mathrm{S} \cdot \left(1 - \frac{\mathrm{P}}{\mathrm{Keq} \cdot \mathrm{S}}\right)}{\mathrm{Ks} \cdot \left(1 + \frac{\mathrm{S}}{\mathrm{Ks}} + \frac{\mathrm{P}}{\mathrm{Kp}}\right)} \tag{87}$$

$$\mathrm{v1sub1prod}(\mathrm{Vfmax}, \mathrm{Keq}, \mathrm{S}, \mathrm{Ks}, \mathrm{P}, \mathrm{Kp}) = \frac{\mathrm{Vfmax} \cdot \mathrm{S} \cdot \left(1 - \frac{\mathrm{P}}{\mathrm{Keq} \cdot \mathrm{S}}\right)}{\mathrm{Ks} \cdot \left(1 + \frac{\mathrm{S}}{\mathrm{Ks}} + \frac{\mathrm{P}}{\mathrm{Kp}}\right)} \tag{88}$$

Table 116: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
PGL_g_Vmax	PGL_g_Vmax		5.000		☑
PGL_g_Keq	PGL_g_Keq		20000.000		☑
PGL_g_Km6PGL	PGL_g_Km6PGL		0.050		☑
PGL_g_Km6PG	PGL_g_Km6PG		0.050		☑
PGL_g_k	PGL_g_k		0.055		☑

6.29 Reaction TR_c

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

Name TR_c

Reaction equation

$$\text{TS2\_c} + \text{NADPH\_c} \xrightleftharpoons{\text{TS2\_c, NADPH\_c, TSH2\_c, NADP\_c}} \text{NADP\_c} + \text{TSH2\_c} \qquad (89)$$

Reactants

Table 117: Properties of each reactant.

Id	Name	SBO
TS2_c	TS2_c	
NADPH_c	NADPH_c	

Modifiers

Table 118: Properties of each modifier.

Id	Name	SBO
TS2_c	TS2_c	
NADPH_c	NADPH_c	
TSH2_c	TSH2_c	
NADP_c	NADP_c	

Products

Table 119: Properties of each product.

Id	Name	SBO
NADP_c	NADP_c	
TSH2_c	TSH2_c	

Kinetic Law

Derived unit contains undeclared units

$$v_{29} = \text{v2sub2prod}\left(\text{TR\_c\_Vmax}, \text{TR\_c\_Keq}, [\text{TS2\_c}], \text{TR\_c\_KmTS2}, [\text{NADPH\_c}], \text{TR\_c\_KmNADPH}, [\text{TSH2\_c}], \text{TR\_c\_KmTSH2}, [\text{NADP\_c}], \text{TR\_c\_KmNADP}\right) \tag{90}$$

$$\text{v2sub2prod}\left(\text{Vfmax}, \text{Keq}, \text{S1}, \text{Ks1}, \text{S2}, \text{Ks2}, \text{P1}, \text{Kp1}, \text{P2}, \text{Kp2}\right) = \frac{\text{Vfmax} \cdot \text{S1} \cdot \text{S2} \cdot \left(1 - \frac{\text{P1} \cdot \text{P2}}{\text{Keq} \cdot \text{S1} \cdot \text{S2}}\right)}{\text{Ks1} \cdot \text{Ks2} \cdot \left(1 + \frac{\text{S1}}{\text{Ks1}} + \frac{\text{P1}}{\text{Kp1}}\right) \cdot \left(1 + \frac{\text{S2}}{\text{Ks2}} + \frac{\text{P2}}{\text{Kp2}}\right)} \tag{91}$$

Table 120: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
TR_c_Vmax	TR_c_Vmax		252.000		☑
TR_c_Keq	TR_c_Keq		434.000		☑
TR_c_KmTS2	TR_c_KmTS2		0.007		☑
TR_c_KmNADPH	TR_c_KmNADPH		$7.7 \cdot 10^{-4}$		☑
TR_c_KmTSH2	TR_c_KmTSH2		0.002		☑
TR_c_KmNADP	TR_c_KmNADP		0.081		☑

6.30 Reaction PGK_g

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

Name PGK_g

Reaction equation

$$\text{\_13BPGA\_g} + \text{ADP\_g} \xrightleftharpoons{\text{\_13BPGA\_g, ADP\_g, \_3PGA\_g, ATP\_g}} \text{\_3PGA\_g} + \text{ATP\_g} \tag{92}$$

Reactants

Table 121: Properties of each reactant.

Id	Name	SBO
_13BPGA_g	_13BPGA_g	
ADP_g	ADP_g	

Modifiers

Table 122: Properties of each modifier.

Id	Name	SBO
_13BPGA_g	_13BPGA_g	
ADP_g	ADP_g	
_3PGA_g	_3PGA_g	
ATP_g	ATP_g	

Products

Table 123: Properties of each product.

Id	Name	SBO
_3PGA_g	_3PGA_g	
ATP_g	ATP_g	

Kinetic Law

Derived unit contains undeclared units

$$v_{30} = \text{v2sub2prod}\,(\text{PGK\_g\_Vmax}, \text{PGK\_g\_Keq}, [\text{\_13BPGA\_g}], \text{PGK\_g\_Km13BPGA}, [\text{ADP\_g}], \text{PGK\_g\_KmADP}, [\text{\_3PGA\_g}], \text{PGK\_g\_Km3PGA}, [\text{ATP\_g}], \text{PGK\_g\_KmATP}) \tag{93}$$

$$\begin{aligned} &\text{v2sub2prod}\,(\text{Vfmax}, \text{Keq}, \text{S1}, \text{Ks1}, \text{S2}, \text{Ks2}, \text{P1}, \text{Kp1}, \text{P2}, \text{Kp2}) \\ &= \frac{\text{Vfmax} \cdot \text{S1} \cdot \text{S2} \cdot \left(1 - \frac{\text{P1} \cdot \text{P2}}{\text{Keq} \cdot \text{S1} \cdot \text{S2}}\right)}{\text{Ks1} \cdot \text{Ks2} \cdot \left(1 + \frac{\text{S1}}{\text{Ks1}} + \frac{\text{P1}}{\text{Kp1}}\right) \cdot \left(1 + \frac{\text{S2}}{\text{Ks2}} + \frac{\text{P2}}{\text{Kp2}}\right)} \end{aligned} \tag{94}$$

Table 124: 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		☑
PGK_g_KmADP	PGK_g_KmADP		0.100		☑
PGK_g_Km3PGA	PGK_g_Km3PGA		1.620		☑
PGK_g_KmATP	PGK_g_KmATP		0.290		☑

6.31 Reaction G3PDH_g

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

Name G3PDH_g

Reaction equation

$$\mathrm{NADH\_g} + \mathrm{DHAP\_g} \xrightleftharpoons{\mathrm{DHAP\_g,\ NADH\_g,\ Gly3P\_g,\ NAD\_g}} \mathrm{Gly3P\_g} + \mathrm{NAD\_g} \qquad (95)$$

Reactants

Table 125: Properties of each reactant.

Id	Name	SBO
NADH_g	NADH_g	
DHAP_g	DHAP_g	

Modifiers

Table 126: Properties of each modifier.

Id	Name	SBO
DHAP_g	DHAP_g	
NADH_g	NADH_g	
Gly3P_g	Gly3P_g	
NAD_g	NAD_g	

Products

Table 127: Properties of each product.

Id	Name	SBO
Gly3P_g	Gly3P_g	
NAD_g	NAD_g	

Kinetic Law

Derived unit contains undeclared units

$$v_{31} = \text{v2sub2prod}\,(\text{G3PDH\_g\_Vmax}, \text{G3PDH\_g\_Keq}, [\text{DHAP\_g}], \text{G3PDH\_g\_KmDHAP}, [\text{NADH\_g}], \text{G3PDH\_g\_KmNADH}, [\text{Gly3P\_g}], \text{G3PDH\_g\_KmGly3P}, [\text{NAD\_g}], \text{G3PDH\_g\_KmNAD}) \quad (96)$$

$$\text{v2sub2prod}\,(\text{Vfmax}, \text{Keq}, \text{S1}, \text{Ks1}, \text{S2}, \text{Ks2}, \text{P1}, \text{Kp1}, \text{P2}, \text{Kp2}) = \frac{\text{Vfmax} \cdot \text{S1} \cdot \text{S2} \cdot \left(1 - \frac{\text{P1} \cdot \text{P2}}{\text{Keq} \cdot \text{S1} \cdot \text{S2}}\right)}{\text{Ks1} \cdot \text{Ks2} \cdot \left(1 + \frac{\text{S1}}{\text{Ks1}} + \frac{\text{P1}}{\text{Kp1}}\right) \cdot \left(1 + \frac{\text{S2}}{\text{Ks2}} + \frac{\text{P2}}{\text{Kp2}}\right)} \quad (97)$$

Table 128: 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		☑

6.32 Reaction ATPu_c

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

Name ATPu_c

Reaction equation

$$\text{ATP\_c} \xrightarrow{\text{ATP\_c, ADP\_c}} \text{ADP\_c} \tag{98}$$

Reactant

Table 129: Properties of each reactant.

Id	Name	SBO
ATP_c	ATP_c	

Modifiers

Table 130: Properties of each modifier.

Id	Name	SBO
ATP_c	ATP_c	
ADP_c	ADP_c	

Product

Table 131: Properties of each product.

Id	Name	SBO
ADP_c	ADP_c	

Kinetic Law

Derived unit contains undeclared units

$$v_{32} = \frac{\text{ATPu\_c\_k} \cdot [\text{ATP\_c}]}{[\text{ADP\_c}]} \tag{99}$$

Table 132: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
ATPu_c_k	ATPu_c_k		50.0		☑

6.33 Reaction GK_g

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

Name GK_g

Reaction equation

$$\text{Gly3P\_g} + \text{ADP\_g} \xrightleftharpoons{\text{Gly3P\_g, ADP\_g, Gly\_e, ATP\_g}} \text{Gly\_e} + \text{ATP\_g} \tag{100}$$

Reactants

Table 133: Properties of each reactant.

Id	Name	SBO
Gly3P_g	Gly3P_g	
ADP_g	ADP_g	

Modifiers

Table 134: Properties of each modifier.

Id	Name	SBO
Gly3P_g	Gly3P_g	
ADP_g	ADP_g	
Gly_e	Gly_e	
ATP_g	ATP_g	

Products

Table 135: Properties of each product.

Id	Name	SBO
Gly_e	Gly_e	
ATP_g	ATP_g	

Kinetic Law

Derived unit contains undeclared units

$$v_{33} = \text{v2sub2prod}\,(\text{GK\_g\_Vmax}, \text{GK\_g\_Keq}, [\text{Gly3P\_g}], \text{GK\_g\_KmGly3P}, [\text{ADP\_g}], \text{GK\_g\_KmADP}, [\text{Gly\_e}], \text{GK\_g\_KmGly}, [\text{ATP\_g}], \text{GK\_g\_KmATP}) \tag{101}$$

$$\begin{aligned}&\text{v2sub2prod}\left(\text{Vfmax}, \text{Keq}, \text{S1}, \text{Ks1}, \text{S2}, \text{Ks2}, \text{P1}, \text{Kp1}, \text{P2}, \text{Kp2}\right)\\ &= \frac{\text{Vfmax} \cdot \text{S1} \cdot \text{S2} \cdot \left(1 - \frac{\text{P1} \cdot \text{P2}}{\text{Keq} \cdot \text{S1} \cdot \text{S2}}\right)}{\text{Ks1} \cdot \text{Ks2} \cdot \left(1 + \frac{\text{S1}}{\text{Ks1}} + \frac{\text{P1}}{\text{Kp1}}\right) \cdot \left(1 + \frac{\text{S2}}{\text{Ks2}} + \frac{\text{P2}}{\text{Kp2}}\right)}\end{aligned} \tag{102}$$

Table 136: 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		☑

6.34 Reaction ALD_g

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

Name ALD_g

Reaction equation

$$\text{Fru16BP\_g} \xrightleftharpoons{\text{ATP\_g, ADP\_g, AMP\_g, Fru16BP\_g, GA3P\_g, DHAP\_g, ATP\_g, ADP\_g, AMP\_g}} \text{GA3P\_g} + \text{DHAP\_g} \tag{103}$$

Reactant

Table 137: Properties of each reactant.

Id	Name	SBO
Fru16BP_g	Fru16BP_g	

Modifiers

Table 138: Properties of each modifier.

Id	Name	SBO
ATP_g	ATP_g	
ADP_g	ADP_g	

Id	Name	SBO
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 139: Properties of each product.

Id	Name	SBO
GA3P_g	GA3P_g	
DHAP_g	DHAP_g	

Kinetic Law

Derived unit contains undeclared units

$$v_{34} \quad (104)$$

$$= \frac{\text{ALD\_g\_V}}{\text{ALD\_g\_KmFru16BP} \cdot \left(1 + \frac{[\text{ATP\_g}]}{\text{ALD\_g\_KiATP}} + \frac{[\text{ADP\_g}]}{\text{ALD\_g\_KiADP}} + \frac{[\text{AMP\_g}]}{\text{ALD\_g\_KiAMP}}\right) \cdot \left(1 + \frac{[\text{GA3P\_g}]}{\text{ALD\_g\_KmGA3P}} + \frac{[\text{DHAP\_g}]}{\text{ALD\_g\_KmDHAP}} +\right.}$$

Table 140: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
ALD_g_Vmax	ALD_g_Vmax		560.000		☑
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		☑

6.35 Reaction GAPDH_g

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

Name GAPDH_g

Reaction equation

$$\mathrm{GA3P\_g} + \mathrm{NAD\_g} + \mathrm{Pi\_g} \xrightleftharpoons{\mathrm{GA3P\_g,\ NAD\_g,\ \_13BPGA\_g,\ NADH\_g}} \mathrm{NADH\_g} + \mathrm{\_13BPGA\_g} \tag{105}$$

Reactants

Table 141: Properties of each reactant.

Id	Name	SBO
GA3P_g	GA3P_g	
NAD_g	NAD_g	
Pi_g	Pi_g	

Modifiers

Table 142: Properties of each modifier.

Id	Name	SBO
GA3P_g	GA3P_g	
NAD_g	NAD_g	
_13BPGA_g	_13BPGA_g	
NADH_g	NADH_g	

Products

Table 143: Properties of each product.

Id	Name	SBO
NADH_g	NADH_g	
_13BPGA_g	_13BPGA_g	

Kinetic Law

Derived unit contains undeclared units

$$v_{35} = \text{v2sub2prod}\,(\text{GAPDH\_g\_Vmax}, \text{GAPDH\_g\_Keq}, [\text{GA3P\_g}], \text{GAPDH\_g\_KmGA3P}, [\text{NAD\_g}], \text{GAPDH\_g\_KmNAD}, [\text{\_13BPGA\_g}], \text{GAPDH\_g\_Km13BPGA}, [\text{NADH\_g}], \text{GAPDH\_g\_KmNADH}) \tag{106}$$

$$\text{v2sub2prod}\,(\text{Vfmax}, \text{Keq}, \text{S1}, \text{Ks1}, \text{S2}, \text{Ks2}, \text{P1}, \text{Kp1}, \text{P2}, \text{Kp2}) = \frac{\text{Vfmax} \cdot \text{S1} \cdot \text{S2} \cdot \left(1 - \frac{\text{P1} \cdot \text{P2}}{\text{Keq} \cdot \text{S1} \cdot \text{S2}}\right)}{\text{Ks1} \cdot \text{Ks2} \cdot \left(1 + \frac{\text{S1}}{\text{Ks1}} + \frac{\text{P1}}{\text{Kp1}}\right) \cdot \left(1 + \frac{\text{S2}}{\text{Ks2}} + \frac{\text{P2}}{\text{Kp2}}\right)} \tag{107}$$

Table 144: 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		☑

6.36 Reaction GPO_c

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

Name GPO_c

Reaction equation

$$\text{Gly3P\_c} \xrightarrow{\text{Gly3P\_c}} \text{DHAP\_c} \tag{108}$$

Reactant

Table 145: Properties of each reactant.

Id	Name	SBO
Gly3P_c	Gly3P_c	

Modifier

Table 146: Properties of each modifier.

Id	Name	SBO
Gly3P_c	Gly3P_c	

Product

Table 147: Properties of each product.

Id	Name	SBO
DHAP_c	DHAP_c	

Kinetic Law

Derived unit contains undeclared units

$$v_{36} = \text{v1sub}\left(\text{GPO\_c\_Vmax}, [\text{Gly3P\_c}], \text{GPO\_c\_KmGly3P}\right) \tag{109}$$

$$\text{v1sub}\left(\text{Vfmax}, \text{S}, \text{Ks}\right) = \frac{\text{Vfmax} \cdot \text{S}}{\text{Ks} \cdot \left(1 + \frac{\text{S}}{\text{Ks}}\right)} \tag{110}$$

Table 148: 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		☑

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 four reactions (as a reactant in ENO_c and as a product in PGAM_c and as a modifier in PGAM_c, ENO_c).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{\_2PGA\_c} = v_5 - v_8 \tag{111}$$

7.2 Species ATP_c

Name ATP_c

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

This species takes part in ten reactions (as a reactant in HXK_c, ATPT_g, ATPu_c and as a product in PYK_c, AK_c and as a modifier in PYK_c, HXK_c, AK_c, ATPT_g, ATPu_c).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{ATP\_c} = v_2 + v_{14} - v_{12} - v_{21} - v_{32} \tag{112}$$

7.3 Species DHAP_c

Name DHAP_c

Initial concentration $2.23132912\ \text{nmol} \cdot \mu\text{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{DHAP\_c} = v_{36} - v_{20} \tag{113}$$

7.4 Species ATP_g

Name ATP_g

Initial concentration $0.2405\ \text{nmol} \cdot \mu\text{l}^{-1}$

This species takes part in 14 reactions (as a reactant in PFK_g, HXK_g and as a product in AK_g, ATPT_g, PGK_g, GK_g and as a modifier in PFK_g, HXK_g, AK_g, ATPT_g, PGK_g, GK_g, ALD_g, ALD_g).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{ATP\_g} = v_{18} + v_{21} + v_{30} + v_{33} - v_3 - v_9 \tag{114}$$

7.5 Species DHAP_g

Name DHAP_g

Initial concentration $8.483130623\ \mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{DHAP\_g} = v_{20} + v_{34} - v_1 - v_{31} \tag{115}$$

7.6 Species ADP_g

Name ADP_g

Initial concentration $1.519\ \mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$

This species takes part in 14 reactions (as a reactant in AK_g, ATPT_g, PGK_g, GK_g and as a product in PFK_g, HXK_g and as a modifier in PFK_g, HXK_g, AK_g, ATPT_g, PGK_g, GK_g, ALD_g, ALD_g).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ADP\_g} = v_3 + v_9 - 2\,v_{18} - v_{21} - v_{30} - v_{33} \tag{116}$$

7.7 Species Glc6P_g

Name Glc6P_g

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

This species takes part in six reactions (as a reactant in G6PDH_g, PGI_g and as a product in HXK_g and as a modifier in G6PDH_g, HXK_g, PGI_g).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Glc6P\_g} = v_9 - v_4 - v_{17} \tag{117}$$

7.8 Species ADP_c

Name ADP_c

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

This species takes part in ten reactions (as a reactant in PYK_c, AK_c and as a product in HXK_c, ATPT_g, ATPu_c and as a modifier in PYK_c, HXK_c, AK_c, ATPT_g, ATPu_c).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ADP\_c} = v_{12} + v_{21} + v_{32} - v_2 - 2\,v_{14} \tag{118}$$

7.9 Species _3PGA_c

Name _3PGA_c

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

This species takes part in four reactions (as a reactant in PGAM_c and as a product in _3PGAT_g and as a modifier in PGAM_c, _3PGAT_g).

$$\frac{\mathrm{d}}{\mathrm{d}t}\_3\mathrm{PGA\_c} = v_{10} - v_5 \tag{119}$$

7.10 Species Fru6P_g

Name Fru6P_g

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

This species takes part in four reactions (as a reactant in PFK_g and as a product in PGI_g and as a modifier in PFK_g, PGI_g).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Fru6P\_g} = v_{17} - v_3 \tag{120}$$

7.11 Species Pi_g

Name Pi_g

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

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:

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

7.12 Species O2_c

Name O2_c

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{O2\_c} = 0 \tag{122}$$

7.13 Species NADP_c

Name NADP_c

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

This species takes part in seven reactions (as a reactant in G6PDH_c, _6PGDH_c and as a product in NADPHu_c, TR_c and as a modifier in G6PDH_c, _6PGDH_c, TR_c).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{NADP\_c} = v_{11} + v_{29} - v_{7} - v_{23} \tag{123}$$

7.14 Species NADP_g

Name NADP_g

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

This species takes part in five reactions (as a reactant in G6PDH_g, _6PGDH_g and as a product in NADPHu_g and as a modifier in G6PDH_g, _6PGDH_g).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{NADP\_g} = v_{13} - v_{4} - v_{16} \tag{124}$$

7.15 Species _6PG_g

Name _6PG_g

Initial concentration $0.0841958\ \mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$

This species takes part in six reactions (as a reactant in _6PGDH_g and as a product in PGL_g and as a modifier in _6PGDH_g, PGI_g, PGI_g, PGL_g).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{\_6PG\_g} = v_{28} - v_{16} \tag{125}$$

7.16 Species CO2_c

Name CO2_c

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

This species takes part in one reaction (as a product in _6PGDH_c), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{CO2\_c} = 0 \tag{126}$$

7.17 Species Ru5P_c

Name Ru5P_c

Initial concentration $0.41282\ \text{nmol} \cdot \mu\text{l}^{-1}$

This species takes part in four reactions (as a reactant in PPI_c and as a product in _6PGDH_c and as a modifier in _6PGDH_c, PPI_c).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{Ru5P\_c} = v_{23} - v_{24} \tag{127}$$

7.18 Species _6PG_c

Name _6PG_c

Initial concentration $0.0841958\ \text{nmol} \cdot \mu\text{l}^{-1}$

This species takes part in four reactions (as a reactant in _6PGDH_c and as a product in PGL_c and as a modifier in PGL_c, _6PGDH_c).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{\_6PG\_c} = v_{22} - v_{23} \tag{128}$$

7.19 Species Ru5P_g

Name Ru5P_g

Initial concentration $0.41282\ \text{nmol} \cdot \mu\text{l}^{-1}$

This species takes part in four reactions (as a reactant in PPI_g and as a product in _6PGDH_g and as a modifier in _6PGDH_g, PPI_g).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{Ru5P\_g} = v_{16} - v_{25} \tag{129}$$

7.20 Species Glc6P_c

Name Glc6P_c

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

This species takes part in six reactions (as a reactant in G6PDH_c, G6PP_c and as a product in HXK_c and as a modifier in G6PDH_c, HXK_c, G6PP_c).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{Glc6P\_c} = v_{12} - v_7 - v_{15} \tag{130}$$

7.21 Species Rib5P_c

Name Rib5P_c

Initial concentration $0.01\ \text{nmol} \cdot \mu\text{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{Rib5P\_c} = 0 \tag{131}$$

7.22 Species _13BPGA_g

Name _13BPGA_g

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{\_13BPGA\_g} = v_{35} - v_{30} \tag{132}$$

7.23 Species Glc_c

Name Glc_c

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

This species takes part in eight reactions (as a reactant in HXK_c, GlcT_g and as a product in G6PP_c, GlcT_c and as a modifier in HXK_c, G6PP_c, GlcT_g, GlcT_c).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{Glc\_c} = v_{15} + v_{27} - v_{12} - v_{26} \tag{133}$$

7.24 Species Rib5P_g

Name Rib5P_g

Initial concentration $0.01\ \text{nmol} \cdot \mu\text{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{Rib5P\_g} = 0 \tag{134}$$

7.25 Species Glc_g

Name Glc_g

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Glc\_g} = v_{26} - v_9 \tag{135}$$

7.26 Species Glc_e

Name Glc_e

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Glc\_e} = 0 \tag{136}$$

7.27 Species NADPH_g

Name NADPH_g

Initial concentration $3.9\ \mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$

This species takes part in six reactions (as a reactant in NADPHu_g and as a product in G6PDH_g, _6PGDH_g and as a modifier in G6PDH_g, NADPHu_g, _6PGDH_g).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{NADPH\_g} = v_4 + v_{16} - v_{13} \tag{137}$$

7.28 Species NADPH_c

Name NADPH_c

Initial concentration $3.9\ \mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$

This species takes part in eight reactions (as a reactant in NADPHu_c, TR_c and as a product in G6PDH_c, _6PGDH_c and as a modifier in G6PDH_c, NADPHu_c, _6PGDH_c, TR_c).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{NADPH\_c} = v_7 + v_{23} - v_{11} - v_{29} \tag{138}$$

7.29 Species Pyr_c

Name Pyr_c

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Pyr\_c} = v_2 - v_6 \tag{139}$$

7.30 Species Pyr_e

Name Pyr_e

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

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:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Pyr\_e} = 0 \tag{140}$$

7.31 Species NAD_g

Name NAD_g

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{NAD\_g} = v_{31} - v_{35} \tag{141}$$

7.32 Species Fru16BP_g

Name Fru16BP_g

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Fru16BP\_g} = v_3 - v_{34} \tag{142}$$

7.33 Species GA3P_g

Name GA3P_g

Initial concentration $2.5\ \mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{GA3P\_g} = v_1 + v_{34} - v_{35} \tag{143}$$

7.34 Species Gly_e

Name Gly_e

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Gly\_e} = 0 \tag{144}$$

7.35 Species TSH2_c

Name TSH2_c

Initial concentration $0.01\ \mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$

This species takes part in four reactions (as a reactant in TOX_c and as a product in TR_c and as a modifier in TOX_c, TR_c).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{TSH2\_c} = v_{29} - v_{19} \tag{145}$$

7.36 Species CO2_g

Name CO2_g

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

This species takes part in one reaction (as a product in _6PGDH_g), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{CO2\_g} = 0 \tag{146}$$

7.37 Species Gly3P_c

Name Gly3P_c

Initial concentration $2.76867088\ \mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Gly3P\_c} = v_{20} - v_{36} \tag{147}$$

7.38 Species Gly3P_g

Name Gly3P_g

Initial concentration $10.51686938\ \mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Gly3P\_g} = v_{31} - v_{20} - v_{33} \tag{148}$$

7.39 Species _6PGL_c

Name _6PGL_c

Initial concentration $0.0795278\ \mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$

This species takes part in four reactions (as a reactant in PGL_c and as a product in G6PDH_c and as a modifier in G6PDH_c, PGL_c).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{\_6PGL\_c} = v_{7} - v_{22} \tag{149}$$

7.40 Species TS2_c

Name TS2_c

Initial concentration $0.37\ \mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$

This species takes part in three reactions (as a reactant in TR_c and as a product in TOX_c and as a modifier in TR_c).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{TS2\_c} = v_{19} - v_{29} \tag{150}$$

7.41 Species _6PGL_g

Name _6PGL_g

Initial concentration $0.0795278\ \text{nmol} \cdot \mu\text{l}^{-1}$

This species takes part in four reactions (as a reactant in PGL_g and as a product in G6PDH_g and as a modifier in G6PDH_g, PGL_g).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{\_6PGL\_g} = v_4 - v_{28} \tag{151}$$

7.42 Species PEP_c

Name PEP_c

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

This species takes part in four reactions (as a reactant in PYK_c and as a product in ENO_c and as a modifier in PYK_c, ENO_c).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{PEP\_c} = v_8 - v_2 \tag{152}$$

7.43 Species AMP_g

Name AMP_g

Initial concentration $4.2405\ \text{nmol} \cdot \mu\text{l}^{-1}$

This species takes part in four reactions (as a product in AK_g and as a modifier in AK_g, ALD_g, ALD_g).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{AMP\_g} = v_{18} \tag{153}$$

7.44 Species _3PGA_g

Name _3PGA_g

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

This species takes part in four reactions (as a reactant in _3PGAT_g and as a product in PGK_g and as a modifier in _3PGAT_g, PGK_g).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{\_3PGA\_g} = v_{30} - v_{10} \tag{154}$$

7.45 Species AMP_c

Name AMP_c

Initial concentration $2.2418\ \mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{AMP\_c} = v_{14} \tag{155}$$

7.46 Species NADH_g

Name NADH_g

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{NADH\_g} = v_{35} - v_{31} \tag{156}$$

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

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