# **SBML Model Report**

# Model name: "Kerkhoven2013 - Glycolysis and Pentose Phosphate Pathway in T.brucei - MODEL C in fructose medium (with glucosomal ribokinase)"



May 5, 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<sup>1</sup> and Eduard Kerkhoven<sup>2</sup> at February tenth 2014 at 2:41 p.m. and last time modified at March fifth 2014 at 4:02 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	51
events	0	constraints	0
reactions	40	function definitions	7
global parameters	0	unit definitions	5
rules	0	initial assignments	0

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#### **Model Notes**

Kerkhoven2013 - Glycolysis and Pentose Phosphate Pathway in T.brucei - MODEL C in fructose medium (with glucosomal ribokinase)

There are six models (Model A, B, C, C-fruc, D, D-fruc) described in the paper. Model A ( BIOMD000000513) 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 C-fruc 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 identified by: BIOMD0000000515.

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  $\mu l$ 

# 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<sup>2</sup>

# 3 Compartments

This model contains three compartments.

Table 2: Properties of all compartments.

	-		permes or air co	p			
Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
cytosol	cytosol	0000290	3	5.4549	μl		
glycosome	glycosome	0000290	3	0.2451	μl	$\overline{\mathbf{Z}}$	
default	default	0000290	3	1	litre	$\overline{\mathbf{Z}}$	

# **3.1 Compartment** cytosol

This is a three dimensional compartment with a constant size of  $5.4549~\mu l$ .

Name cytosol

SBO:0000290 physical compartment

# 3.2 Compartment glycosome

This is a three dimensional compartment with a constant size of 0.2451  $\mu l.$ 

Name glycosome

**SBO:0000290** physical compartment

# 3.3 Compartment default

This is a three dimensional compartment with a constant size of one  $\mu l$ .

Name default

SBO:0000290 physical compartment

# 4 Species

This model contains 51 species. The boundary condition of eleven 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
Fru_e	Fru_e	default	$nmol \cdot \mu l^{-1}$		$\overline{Z}$
_2PGA_c	_2PGA_c	cytosol	$nmol \cdot \mu l^{-1}$		
Fru_g	Fru_g	glycosome	$nmol \cdot \mu l^{-1}$		
$Fru_c$	Fru_c	cytosol	$nmol \cdot \mu l^{-1}$		
DHAP_c	DHAP_c	cytosol	$nmol \cdot \mu l^{-1}$		
$ATP_g$	ATP_g	glycosome	$nmol \cdot \mu l^{-1}$		
DHAP_g	DHAP_g	glycosome	$nmol \cdot \mu l^{-1}$		
$ADP_g$	$ADP_{-}g$	glycosome	$nmol \cdot \mu l^{-1}$		
Glc6P_g	Glc6P_g	glycosome	$nmol \cdot \mu l^{-1}$		
$ADP_c$	$ADP_{-}c$	cytosol	$nmol \cdot \mu l^{-1}$		
_3PGA_c	_3PGA_c	cytosol	$nmol \cdot \mu l^{-1}$		
NADPH_c	NADPH_c	cytosol	$nmol \cdot \mu l^{-1}$		
Fru6P_g	Fru6P_g	glycosome	$nmol \cdot \mu l^{-1}$		
Fru6P_c	Fru6P_c	cytosol	$nmol \cdot \mu l^{-1}$		
Pi_g	Pi_g	glycosome	nmol $\cdot \mu l^{-1}$		
02_c	$O2_c$	default	$nmol \cdot \mu l^{-1}$		
$NADP_c$	$NADP_c$	cytosol	$nmol \cdot \mu l^{-1}$		
$ATP_c$	ATP_c	cytosol	$nmol \cdot \mu l^{-1}$		
NADP_g	NADP_g	glycosome	$nmol \cdot \mu l^{-1}$		
_6PG_g	_6PG_g	glycosome	$nmol \cdot \mu l^{-1}$		
CO2_c	CO2_c	cytosol	$nmol \cdot \mu l^{-1}$		

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6	Id	Name	Compartment	Derived Unit	Constant	Boundary Condi- tion
	Rul5P_c	Rul5P_c	cytosol	$nmol \cdot \mu l^{-1}$		
	_6PG_c	_6PG_c	cytosol	$nmol \cdot \mu l^{-1}$		
	Rul5P_g	Rul5P_g	glycosome	$nmol \cdot \mu l^{-1}$		
	${\tt Glc6P\_c}$	Glc6P_c	cytosol	$nmol \cdot \mu l^{-1}$		
	$Rib5P_c$	Rib5P_c	cytosol	$nmol \cdot \mu l^{-1}$		
	$_{ m L}$ 13BPGA $_{ m L}$ g	_13BPGA_g	glycosome	$nmol \cdot \mu l^{-1}$		
	${ t Glc\_c}$	Glc_c	cytosol	$nmol \cdot \mu l^{-1}$		
	$Rib5P_g$	Rib5P_g	glycosome	$nmol \cdot \mu l^{-1}$		
$r_0$	${ t Glc\_g}$	Glc_g	glycosome	$nmol \cdot \mu l^{-1}$		
duc	${ t Glc_e}$	Glc_e	default	$nmol \cdot \mu l^{-1}$		
ed	$NADPH_g$	$NADPH_{-}g$	glycosome	$nmol \cdot \mu l^{-1}$		
by	$\mathtt{Rib}_{\mathtt{g}}$	Rib_g	glycosome	$nmol \cdot \mu l^{-1}$		
Produced by SBML216TEX	$Pyr_{-}c$	Pyr_c	cytosol	$n \text{mol} \cdot \mu l^{-1}$		
<u>≦</u>	$Pyr_{-}e$	Pyr_e	default	$n \text{mol} \cdot \mu l^{-1}$		
Ä	$NAD_g$	$NAD_{-g}$	glycosome	$n \text{mol} \cdot \mu l^{-1}$	$\Box$	$\Box$
'×	Fru16BP_g	Fru16BP_g	glycosome	$nmol \cdot \mu l^{-1}$	$\Box$	$\Box$
	$GA3P_g$	GA3P_g	glycosome	$nmol \cdot \mu l^{-1}$	$\Box$	$\Box$
	${ t Gly_e}$	$Gly_e$	default	$nmol \cdot \mu l^{-1}$		
	TSH2_c	TSH2_c	cytosol	$n \text{mol} \cdot \mu l^{-1}$	$\Box$	$\Box$
	CO2_g	CO2_g	glycosome	$nmol \cdot \mu l^{-1}$		
	${\tt Gly3P\_c}$	Gly3P_c	cytosol	$nmol \cdot \mu l^{-1}$		$\Box$
	Gly3P_g	Gly3P_g	glycosome	$nmol \cdot \mu l^{-1}$	$\Box$	$\Box$
	_6PGL_c	_6PGL_c	cytosol	$nmol \cdot \mu l^{-1}$	$\Box$	$\Box$
	$TS2_c$	TS2_c	cytosol	$nmol \cdot \mu l^{-1}$	$\Box$	
	$_{ t 6}$ PGL $_{ t g}$	_6PGL_g	glycosome	$nmol \cdot \mu l^{-1}$		
	$PEP_c$	PEP_c	cytosol	$nmol \cdot \mu l^{-1}$	$\Box$	$\Box$
	$\mathtt{AMP}_{-}\!\mathtt{g}$	$AMP_{-}g$	glycosome	$nmol \cdot \mu l^{-1}$		

Id	Name	Compartment	Derived Unit	Constant	Boundary Condi- tion
_3PGA_g	_3PGA_g	glycosome	$nmol \cdot \mu l^{-1}$		
AMP_c	$AMP_c$	cytosol	$nmol \cdot \mu l^{-1}$		
$NADH_g$	$NADH_g$	glycosome	$nmol \cdot \mu l^{-1}$	$\Box$	$\Box$

## 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** 

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

#### 5.3 Function definition v1sub

Name v1sub

Arguments Vfmax, S, Ks

**Mathematical Expression** 

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

#### 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** 

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

#### 5.5 Function definition mass\_action\_rev

Name mass\_action\_rev

Arguments k1, S, k2, P

**Mathematical Expression** 

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

# 5.6 Function definition v1sub1prod

Name v1sub1prod

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

**Mathematical Expression** 

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

# **5.7 Function definition** mass\_action\_irrev

Name mass\_action\_irrev

 $\textbf{Arguments} \ k, S \\$ 

**Mathematical Expression** 

$$\mathbf{k} \cdot \mathbf{S}$$
 (7)

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# 6 Reactions

This model contains 40 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

		140	one 4. Overview of all feactions	
No	Id	Name	Reaction Equation SBO	
1	TPI_g	TPI_g	DHAP_g DHAP_g, GA3P_g GA3P_g	
2	PYK_c	PYK_c	$PEP_c + ADP_c \xrightarrow{ADP_c, Pyr_c, ATP_c, PEP_c} Pyr_c +$	
			ATP_c	
3	PFK_g	PFK_g	$ATP_g + Fru6P_g \xrightarrow{Fru6P_g, ATP_g, Fru16BP_g, ADP_g} Fru16BP_g$	g+
	<u> </u>		ADP_g	
4	G6PDH_g	$G6PDH_{-g}$	$Glc6Pg + NADPg \xrightarrow{Glc6Pg, NADPg, \_6PGLg, NADPHg} \_6PGLg$	$\mathrm{GL}_{\sigma}$
_	dol bli_g	GOI DIII-g	NADPH_g	3D-5
5	PGAM_c	PGAM_c	_3PGA_c = 3PGA_c, _2PGA_c _2PGA_c	
3	FGAPI_C	I GAWLC	·	
6	PyrT_c	PyrT_c	$Pyr_c \xrightarrow{Pyr_c} Pyr_e$	
7	G6PDH_c	$G6PDH_{-}c$	$Glc6P_c+NADP_c \xrightarrow{Glc6P_c, NADP_c, \_6PGL_c, NADPH_c} NADP_c$	PH_c+
			_6PGL_c	
8	ENO_c	ENO_c	_2PGA_c = PEP_c PEP_c	
Ü			Fru_g, Fru6P_g, Glc_g, ATP_g, Glc6P_g, ADP_g, F	ru_g, Fru6P_g
9	$HXK_g$	$HXK_{-g}$		
			ADP_g	
10	RK_g	RK_g	$ADPg + Rib5Pg$ $\xrightarrow{Rib5Pg, ADPg, Ribg, ATPg}$ $ATPg +$	
	3	<u> </u>	Rib_g	
11	_3PGAT_g	_3PGAT_g	_3PGA_g =	
11	_or gwr_g	_31 GA1 _g	21 GA_g	

	N⁰	Id	Name	Reaction Equation SBO	
	12	${\tt NADPHu\_c}$	NADPHu_c	$NADPH_c \xrightarrow{NADPH_c} NADP_c$	
	13	$HXK_{-}c$	HXK_c	Glc_c+ATP_c Fru_c, Fru6P_c, Glc_c, ATP_c, Glc6P_c, ADP_c, Fru_c, Fru6P_c	$\stackrel{\text{2-c}}{\Longrightarrow}$ Glc6P_
				ADP_c	
	14	${\tt NADPHu\_g}$	NADPHu_g	$NADPH\_g \xrightarrow{NADPH\_g} NADP\_g$	
	15	$\mathtt{HXKfru}_{\mathtt{g}}$	$HXKfru_{-}g$	Fru_g + ATP_g Clc_g, Glc6P_g, Fru_g, ATP_g, Fru6P_g, ADP_g, Glc_g, Glc6P_g, Fru6P_g	$\stackrel{\text{5P-g}}{=\!=\!=} ADP.$
	16	G6PP_c	G6PP_c	Glc6P_c Glc6P_c, Glc_c Glc_c	
Pro	17	AK_c	AK_c	$2 \text{ ADP\_c} \xrightarrow{\text{ADP\_c}, \text{ AMP\_c}, \text{ ATP\_c}} \text{AMP\_c} + \text{ATP\_c}$	
Produced by SBML2PTEX	18	PGI_g	$PGI_{-g}$	Glc6P-g Glc6P-g, Fru6P-g, _6PG-g Fru6P-g Fru6P-g	0
l by	19	${\tt HXKfru\_c}$	HXKfru_c	Fru_c+ATP_c Glc_c, Glc6P_c, Fru_c, ATP_c, Fru6P_c, ADP_c, Glc_c, Glc6P_c	$\stackrel{?\_c}{\Longrightarrow}$ ADP_c
88				Fru6P_c	
	20	TOX_c	$TOX_c$	$TSH2\_c \xrightarrow{TSH2\_c} TS2\_c$	
Ž	21	$\mathtt{GDA}_{-}\mathtt{g}$	$\mathrm{GDA}_{-\mathrm{g}}$	$Gly3P\_g + DHAP\_c \xrightarrow{Gly3P\_g, DHAP\_c, Gly3P\_c, DHAP\_g} Gly3P\_c +$	
				DHAP_g	
	22	FruT_g	FruT_g	Fru_c, Fru_g Fru_g	
	23	PGL_c	PGL_c	_6PGL_c <u>-6PGL_c</u> , <u>-6PG_c</u> _6PG_c	
	24	FruT_c	FruT_c	$Fru_e \xrightarrow{Fru_e, Fru_c} Fru_c$	
	25	$AK_{-}g$	AK_g	$2 \text{ ADP-g} \stackrel{\text{ADP-g, AMP-g, ATP-g}}{\longleftarrow} \text{AMP-g + ATP-g}$	
	26	_6PGDH_c	_6PGDH_c	NADP_c+_6PG_c = 6PG_c, NADP_c, Rul5P_c, NADPH_c CO2_c+	
11	27	PPI_c	PPI_c	$NADPH_c + Rul5P_c$ $Rul5P_c \xrightarrow{Rul5P_c, Rib5P_c} Rib5P_c$	

12	No	Id	Name	Reaction Equation	SBO
	28	PPI_g	PPI_g	$Rul5P\_g \xrightarrow{Rul5P\_g, Rib5P\_g} Rib5P\_g$	
	29	_6PGDH_g	_6PGDH_g	_6PG_g + NADP_g	PH_g Rul5P_g+
	30	GlcT_g	GlcT_g	$Glc\_c \xrightarrow{Glc\_c, Glc\_g} Glc\_g$	
	31	${\tt GlcT\_c}$	GlcT_c	$Glc\_e \xrightarrow{Glc\_e, Glc\_c} Glc\_c$	
	32	PGL_g	PGL_g	_6PGL_g = _6PGL_g, _6PG_g _6PG_g _6PG_g _7S2 a NADBH a TSH2 a NADBH	D a
$P_T$	33	TR_c	TR_c	TS2_c+NADPH_c TS2_c, NADPH_c, TSH2_c, NAD	$\stackrel{P\_C}{\Longrightarrow}$ NADP_c+
Produced by SBML2LATEX	34	$PGK_{-}g$	PGK_g	TSH2_c _13BPGA_g, ADP_g, _3PGA_g, ATP_g	•
SBMIZ	35	G3PDH_g	G3PDH_g	NADH_g+DHAP_g DHAP_g, NADH_g, Gly3P_g, N NAD_g	$\frac{AD_{g}}{}$ Gly3P_g+
Ā <sub>C</sub>	36	$\mathtt{ATPu\_c}$	ATPu_c	$ATP\_c \xrightarrow{ATP\_c, ADP\_c} ADP\_c$	
	37	GK_g	GK_g	$Gly3P\_g + ADP\_g \xrightarrow{Gly3P\_g, ADP\_g, Gly\_e, ATP\_g} Gl$ $ATP\_g$	ly_e+
	38	ALD_g	ALD_g	Fru16BP_g ATP_g, ADP_g, AMP_g, Fru16BP_g, GA3 DHAP_g	BP_g, DHAP_g, ATP_g, ADP_
	39	GAPDH_g	$GAPDH_{-g}$	GA3P_g + NAD_g +  Pi_g GA3P_g, NAD_g, _13BPGA_g, NADH_g NADH	<b>[</b> σ+
				_13BPGA_g	· 0
	40	GPO_c	GPO_c	$Gly3P_c \xrightarrow{Gly3P_c} DHAP_c$	

# **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**

$$DHAP\_g \xrightarrow{DHAP\_g, GA3P\_g} GA3P\_g$$
 (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 GA3P_g	

#### **Product**

Table 7: Properties of each product.

Id	Name	SBO
GA3P_g	GA3P_g	

#### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_1 = v1sub1prod(TPI\_g\_Vmax, TPI\_g\_Keq, [DHAP\_g], TPI\_g\_KmDHAP, [GA3P\_g], TPI\_g\_KmGA3P)$$
 (9)

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

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		$\overline{\mathbf{Z}}$
$\mathtt{TPI\_g\_KmDHAP}$	$TPI_g_KmDHAP$		1.200		
${\tt TPI\_g\_KmGA3P}$	TPI_g_KmGA3P		0.250		$\checkmark$

# 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**

$$PEP_{c} + ADP_{c} \xrightarrow{ADP_{c}, Pyr_{c}, ATP_{c}, PEP_{c}} Pyr_{c} + ATP_{c}$$

$$(11)$$

#### **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	
$Pyr_{-}c$	$Pyr_{-}c$	
$\mathtt{ATP}_{-}\mathtt{c}$	$ATP_c$	
$PEP_c$	PEP_c	

#### **Products**

Table 11: Properties of each product.

Id	Name	SBO
Pyr_c ATP_c	Pyr_c ATP_c	

**Derived unit** contains undeclared units

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

Table 12: Properties of each parameter.

		1	1		
Id	Name	SBO	Value	Unit	Constant
PYK_c_Vmax	PYK_c_Vmax		1020.000		
$PYK_c_KmPEP$	PYK_c_KmPEP		0.340		$ \overline{\mathbf{Z}} $
PYK_c_KiATP	PYK_c_KiATP		0.570		$\square$
$PYK_c_KiADP$	PYK_c_KiADP		0.640		$\square$
PYK_c_n	PYK_c_n		2.500		$\square$
$PYK_c_KmADP$	PYK_c_KmADP		0.114		$\square$
PYK_c_Keq	PYK_c_Keq		10800.000		$\square$
PYK_c_KmPyr	PYK_c_KmPyr		50.000		$\square$
${\tt PYK\_c\_KmATP}$	PYK_c_KmATP		15.000		$\square$

# 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**

$$ATP\_g + Fru6P\_g \xrightarrow{Fru6P\_g, ATP\_g, Fru16BP\_g, ADP\_g} Fru16BP\_g + ADP\_g \qquad (13)$$

# 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	
$\mathtt{ATP}_{-}\mathtt{g}$	$ATP_{-}g$	
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

$$v_{3} = \frac{PFK\_g\_Vmax \cdot PFK\_g\_Ki1 \cdot [Fru6P\_g] \cdot [ATP\_g] \cdot \left(1 - \frac{[Fru6P\_g]}{PFK\_g\_KmFru6P} \cdot PFK\_g\_KmATP \cdot ([Fru16BP\_g] + PFK\_g\_Ki1) \cdot \left(\frac{PFK\_g\_KsATP}{PFK\_g\_KmATP} + \frac{[Fru6P\_g]}{PFK\_g\_KmFru6P} + \frac{[ATP\_g]}{PFK\_g\_KmATP} + \frac{[ATP\_g]}{PFK\_g\_KmATP} + \frac{[ATP\_g]}{PFK\_g\_KmFru6P} + \frac{[ATP\_g]}{PFK\_g\_KmATP} + \frac{[ATP\_g]}{PFK_g\_KmATP} + \frac{[ATP\_g]}{PFK_g\_g\_KmATP} + \frac{[ATP\_g]}{PFK_g\_g\_KmATP} + \frac{[ATP\_g]}{PFK_g\_g\_KmATP} + \frac{[ATP\_g]}{PFK_g\_g\_KmATP} + \frac{[ATP\_g]}{PFK_g\_$$

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-	PFK_g_KmFru6P		0.999		
_KmFru6P					

Id	Name	SBO	Value	Unit	Constant
PFK_g_KmATP	PFK_g_KmATP		0.065		$\square$
$PFK_g_Keq$	PFK_g_Keq		1035.000		$\mathbf{Z}$
PFK_g_KsATP	PFK_g_KsATP		0.039		
$PFK_g_KmADP$	PFK_g_KmADP		1.000		
PFK_g_Ki2	PFK_g_Ki2		10.700		$\square$

# **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**

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

#### **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	
$NADP_g$	$NADP_{-}g$	
$_{\rm -6PGL\_g}$	_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	

**Derived unit** contains undeclared units

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

$$v2sub2prod (Vfmax, Keq, S1, Ks1, S2, Ks2, P1, Kp1, P2, Kp2) = \frac{Vfmax \cdot S1 \cdot S2 \cdot \left(1 - \frac{P1 \cdot P2}{Keq \cdot S1 \cdot S2}\right)}{Ks1 \cdot Ks2 \cdot \left(1 + \frac{S1}{Ks1} + \frac{P1}{Kp1}\right) \cdot \left(1 + \frac{S2}{Ks2} + \frac{P2}{Kp2}\right)}$$
(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-	G6PDH_g-		0.058		$\square$
$_{\tt KmGlc6P}$	_KmGlc6P				
G6PDH_g-	G6PDH_g-		0.009		
_KmNADP	_KmNADP				
G6PDH_g-	G6PDH_g-		0.040		$\mathbf{Z}$
$_{ m Km6PGL}$	_Km6PGL				
G6PDH_g-	G6PDH_g-		$10^{-4}$		$\square$
_KmNADPH	_KmNADPH				

#### 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**

$$_3PGA_c \stackrel{3PGA_c, _2PGA_c}{\longleftarrow} _2PGA_c$$
 (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

$$v_5 = v1sub1prod (PGAM\_c\_Vmax, PGAM\_c\_Keq, [\_3PGA\_c], PGAM\_c\_Km3PGA, \\ [\_2PGA\_c], PGAM\_c\_Km2PGA)$$
 (19)

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

Table 24: Properties of each parameter.

		•			
Id	Name	SBO	Value	Unit	Constant
PGAM_c_Vmax	PGAM_c_Vmax		225.00		lacksquare
$PGAM_c_Keq$	PGAM_c_Keq		0.17		
PGAM_c-	PGAM_c-		0.15		
_Km3PGA	_Km3PGA				

Id	Name	SBO	Value	Unit	Constant
PGAM_c- _Km2PGA	PGAM_c- _Km2PGA		0.16		Ø

# **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**

$$Pyr_{-}c \xrightarrow{Pyr_{-}c} Pyr_{-}e \tag{21}$$

#### 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

$$v_6 = v1sub(PyrT_c\_Vmax, [Pyr\_c], PyrT_c\_KmPyr)$$
 (22)

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

Table 28: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
PyrT_c_Vmax	PyrT_c_Vmax		230.00		$ \mathbf{Z} $
$PyrT_c_KmPyr$	PyrT_c_KmPyr		1.96		$\overline{\mathbf{Z}}$

#### **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**

$$Glc6P\_c + NADP\_c \xrightarrow{Glc6P\_c, NADP\_c, \_6PGL\_c, NADPH\_c} NADPH\_c + \_6PGL\_c \qquad (24)$$

#### **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	

**Derived unit** contains undeclared units

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

$$v2sub2prod(Vfmax, Keq, S1, Ks1, S2, Ks2, P1, Kp1, P2, Kp2)$$

$$= \frac{Vfmax \cdot S1 \cdot S2 \cdot \left(1 - \frac{P1 \cdot P2}{Keq \cdot S1 \cdot S2}\right)}{Ks1 \cdot Ks2 \cdot \left(1 + \frac{S1}{Ks1} + \frac{P1}{Kp1}\right) \cdot \left(1 + \frac{S2}{Ks2} + \frac{P2}{Kp2}\right)}$$
(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		$\square$
G6PDH_c-	G6PDH_c-		0.058		$\square$
_KmGlc6P	_KmGlc6P				
G6PDH_c-	G6PDH_c-		0.009		$\square$
_KmNADP	_KmNADP				
G6PDH_c-	G6PDH_c-		0.040		$\square$
$_{\tt Km6PGL}$	_Km6PGL				
G6PDH_c-	G6PDH_c-		$10^{-4}$		$\square$
_KmNADPH	_KmNADPH				

## 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**

$$_{2}PGA_{c} \xrightarrow{2PGA_{c}, PEP_{c}} PEP_{c}$$
 (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

$$v_8 = v1sub1prod (ENO\_c\_Vmax, ENO\_c\_Keq, [\_2PGA\_c], ENO\_c\_Km2PGA, [PEP\_c], ENO\_c\_KmPEP)$$

$$(28)$$

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

Table 36: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
ENO_c_Vmax	ENO_c_Vmax		598.000		$   \sqrt{} $
$ENO\_c\_Keq$	ENO_c_Keq		4.170		
${\tt ENO\_c\_Km2PGA}$	ENO_c_Km2PGA		0.054		
${\tt ENO\_c\_KmPEP}$	ENO_c_KmPEP		0.240		$\square$

# **6.9 Reaction HXK\_g**

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

Name  $HXK_{-}g$ 

# **Reaction equation**

$$ATP\_g + Glc\_g \xrightarrow{Fru\_g, Fru6P\_g, Glc\_g, ATP\_g, Glc6P\_g, ADP\_g, Fru\_g, Fru6P\_g} Glc6P\_g + ADP\_g \tag{30}$$

#### **Reactants**

Table 37: Properties of each reactant.

Id	Name	SBO
ATP_g	ATP_g	
${\tt Glc\_g}$	$Glc_{-}g$	

## **Modifiers**

Table 38: Properties of each modifier.

Id	Name	SBO
Fru_g	Fru_g	
Fru6P_g	Fru6P_g	
${\tt Glc\_g}$	Glc_g	
$\mathtt{ATP}_{-}\mathtt{g}$	$ATP_{-}g$	
${\tt Glc6P\_g}$	Glc6P_g	
$ADP_g$	$ADP_{-}g$	
$Fru\_g$	$Fru\_g$	
Fru6P_g	Fru6P_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

v2sub2prod\_compinhib (Vfmax, Keq, S1, Ks1, S2, Ks2, P1, Kp1, P2, Kp2, I1, Ki1, I2, Ki2)

$$= \frac{V f max \cdot S1 \cdot S2 \cdot \left(1 - \frac{P1 \cdot P2}{Keq \cdot S1 \cdot S2}\right)}{Ks1 \cdot Ks2 \cdot \left(1 + \frac{S1}{Ks1} + \frac{P1}{Kp1}\right) \cdot \left(1 + \frac{S2}{Ks2} + \frac{P2}{Kp2} + \frac{I1}{Ki1} + \frac{I2}{Ki2}\right)}$$
(32)

Table 40: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
HXK_g_Vmax	HXK_g_Vmax		1774.680		<b>✓</b>
$HXK_g_Keq$	HXK_g_Keq		759.000		$ \overline{\mathbf{Z}} $
$HXK_g_KmGlc$	HXK_g_KmGlc		0.100		$   \overline{\mathscr{L}} $
$HXK_g_KmATP$	HXK_g_KmATP		0.116		$\overline{\mathbf{Z}}$
HXK_g-	HXK_g_KmGlc6P		2.700		$\overline{\mathbf{Z}}$
$_{\tt KmGlc6P}$					
$HXK_g_KmADP$	HXK_g_KmADP		0.126		
HXK_g_KiFru	HXK_g_KiFru		0.350		$\overline{\mathbf{Z}}$
HXK_g-	HXK_g_KiFru6P		2.700		$ \overline{\mathbf{Z}} $
_KiFru6P					

# 6.10 Reaction RK\_g

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

Name  $RK_{-}g$ 

## **Reaction equation**

$$ADP_{-g} + Rib5P_{-g} \xrightarrow{Rib5P_{-g}, ADP_{-g}, Rib_{-g}, ATP_{-g}} ATP_{-g} + Rib_{-g}$$
 (33)

#### **Reactants**

Table 41: Properties of each reactant.

Id	Name	SBO
ADP_g	ADP_g	
$Rib5P_g$	Rib5P_g	

#### **Modifiers**

Table 42: Properties of each modifier.

Id	Name	SBO
Rib5P_g	Rib5P_g	
$ADP_g$	$ADP_{-}g$	
$Rib\_g$	Rib_g	
ATP_g	ATP_g	

#### **Products**

Table 43: Properties of each product.

P_g D_g

#### **Kinetic Law**

Derived unit contains undeclared units

$$v_{10} = v2sub2prod\left(RK_{g}Vmax, RK_{g}Keq, [Rib5P_{g}], RK_{g}KmRib5P, [ADP_{g}], RK_{g}KmADP, [Rib_{g}], RK_{g}KmRib, [ATP_{g}], RK_{g}KmATP\right)$$
(34)

$$v2sub2prod (Vfmax, Keq, S1, Ks1, S2, Ks2, P1, Kp1, P2, Kp2) = \frac{Vfmax \cdot S1 \cdot S2 \cdot \left(1 - \frac{P1 \cdot P2}{Keq \cdot S1 \cdot S2}\right)}{Ks1 \cdot Ks2 \cdot \left(1 + \frac{S1}{Ks1} + \frac{P1}{Kp1}\right) \cdot \left(1 + \frac{S2}{Ks2} + \frac{P2}{Kp2}\right)}$$
(35)

Table 44: Properties of each parameter.

		1			
Id	Name	SBO	Value	Unit	Constant
RK_g_Vmax	RK_g_Vmax		10.000		
$RK_g_Keq$	RK_g_Keq		0.004		
$RK_g_KmRib5P$	RK_g_KmRib5P		0.390		
$RK_g_KmADP$	$RK_g_KmADP$		0.250		
$RK_g_KmRib$	$RK_{g}_{KmRib}$		0.510		$\square$
$RK_g_KmATP$	$RK_{-}g_{-}KmATP$		0.240		

# **6.11 Reaction** \_3PGAT\_g

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

Name \_3PGAT\_g

# **Reaction equation**

$$_3PGA_g \xrightarrow{_3PGA_g, _3PGA_c} _3PGA_c$$
 (36)

#### 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_c	_3PGA_g _3PGA_c	

# **Product**

Table 47: Properties of each product.

Id	Name	SBO
_3PGA_c	_3PGA_c	

#### Derived unit contains undeclared units

$$v_{11} = \text{mass\_action\_rev} \left( -3\text{PGAT\_g\_k}, [-3\text{PGA\_g}], -3\text{PGAT\_g\_k}, [-3\text{PGA\_c}] \right)$$
 (37)

mass\_action\_rev 
$$(k1, S, k2, P) = k1 \cdot S - k2 \cdot P$$
 (38)

Table 48: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
_3PGAT_g_k	_3PGAT_g_k	250.0	$ \overline{\checkmark} $

# 6.12 Reaction NADPHu\_c

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

#### Name NADPHu\_c

# **Reaction equation**

$$NADPH_c \xrightarrow{NADPH_c} NADP_c$$
 (39)

#### Reactant

Table 49: Properties of each reactant.

Id	Name	SBO
NADPH_c	NADPH_c	

#### **Modifier**

Table 50: Properties of each modifier.

Id	Name	SBO
NADPH_c	NADPH_c	

#### **Product**

Table 51: Properties of each product.

Id	Name	SBO
NADP_c	NADP_c	

**Derived unit** contains undeclared units

$$v_{12} = \text{mass\_action\_irrev} (\text{NADPHu\_c\_k}, [\text{NADPH\_c}])$$
 (40)

$$mass\_action\_irrev\left(k,S\right) = k \cdot S \tag{41}$$

Table 52: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
NADPHu_c_k	NADPHu_c_k	2.0	

# 6.13 Reaction HXK\_c

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

#### Name HXK\_c

## **Reaction equation**

$$Glc\_c + ATP\_c \xrightarrow{Fru\_c, Fru6P\_c, Glc\_c, ATP\_c, Glc6P\_c, ADP\_c, Fru\_c, Fru6P\_c} Glc6P\_c + ADP\_c \tag{42}$$

# **Reactants**

Table 53: Properties of each reactant.

Id	Name	SBO
Glc_c	Glc_c	
$\mathtt{ATP}_{-}\mathtt{c}$	$ATP\_c$	

#### **Modifiers**

Table 54: Properties of each modifier.

Id	Name	SBO
Fru_c	Fru_c	
$Fru6P_c$	Fru6P_c	
${\tt Glc\_c}$	Glc_c	
$ATP_c$	ATP_c	
${\tt Glc6P\_c}$	Glc6P_c	
$ADP_c$	$ADP_c$	
$Fru_c$	Fru_c	
Fru6P_c	Fru6P_c	

#### **Products**

Table 55: Properties of each product.

Id	Name	SBO
Glc6P_c	Glc6P_c	
$ADP_c$	$ADP_c$	

#### **Kinetic Law**

#### Derived unit contains undeclared units

 $v2sub2prod\_compinhib \\ (Vfmax, Keq, S1, Ks1, S2, Ks2, P1, Kp1, P2, Kp2, I1, Ki1, I2, Ki2) \\$ 

$$= \frac{V f max \cdot S1 \cdot S2 \cdot \left(1 - \frac{P1 \cdot P2}{Keq \cdot S1 \cdot S2}\right)}{Ks1 \cdot Ks2 \cdot \left(1 + \frac{S1}{Ks1} + \frac{P1}{Kp1}\right) \cdot \left(1 + \frac{S2}{Ks2} + \frac{P2}{Kp2} + \frac{I1}{Ki1} + \frac{I2}{Ki2}\right)}$$
(44)

Table 56: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
HXK_c_Vmax	HXK_c_Vmax		154.320		<b>✓</b>
$HXK_c_Keq$	$HXK_{-}c_{-}Keq$		759.000		
$\tt HXK\_c\_KmGlc$	$HXK_{-}c_{-}KmGlc$		0.100		$\checkmark$

Id	Name	SBO	Value	Unit	Constant
HXK_c_KmATP HXK_cKmGlc6P	HXK_c_KmATP HXK_c_KmGlc6P		0.116 2.700		<b>1 1</b>
HXK_c_KmADP HXK_c_KiFru HXK_cKiFru6P	HXK_c_KmADP HXK_c_KiFru HXK_c_KiFru6P		0.126 0.350 2.700		

# **6.14 Reaction** NADPHu\_g

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

Name  $NADPHu_g$ 

# **Reaction equation**

$$NADPH_{-}g \xrightarrow{NADPH_{-}g} NADP_{-}g \tag{45}$$

#### Reactant

Table 57: Properties of each reactant.

Id	Name	SBO
NADPH_g	NADPH_g	

#### **Modifier**

Table 58: Properties of each modifier.

Id	Name	SBO
NADPH_g	NADPH_g	

# **Product**

Table 59: Properties of each product.

Id	Name	SBO
NADP_g	NADP_g	

#### **Derived unit** contains undeclared units

$$v_{14} = \text{mass\_action\_irrev} (\text{NADPHu\_g\_k}, [\text{NADPH\_g}])$$
 (46)

$$mass\_action\_irrev(k, S) = k \cdot S$$
 (47)

Table 60: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
NADPHu_g_k	NADPHu_g_k	2.0	

# 6.15 Reaction HXKfru\_g

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

Name HXKfru\_g

# **Reaction equation**

$$Fru\_g + ATP\_g \xrightarrow{Glc\_g, \ Glc6P\_g, \ Fru\_g, \ ATP\_g, \ Fru6P\_g, \ ADP\_g, \ Glc\_g, \ Glc6P\_g} ADP\_g + Fru6P\_g \tag{48}$$

## **Reactants**

Table 61: Properties of each reactant.

Id	Name	SBO
Fru_g	Fru_g	
$ATP_{-}g$	$ATP_{-}g$	

#### **Modifiers**

Table 62: Properties of each modifier.

Id	Name	SBO
Glc_g	Glc_g	
${\tt Glc6P\_g}$	Glc6P_g	
$Fru\_g$	Fru_g	
$ATP_g$	$ATP_{-}g$	

Id	Name	SBO
Fru6P_g	Fru6P_g	
$ADP_g$	$ADP_{-}g$	
${ t Glc\_g}$	Glc_g	
Glc6P_g	Glc6P_g	

#### **Products**

Table 63: Properties of each product.

Id	Name	SBO
ADP_g Fru6P_g	ADP_g Fru6P_g	

#### **Kinetic Law**

#### **Derived unit** contains undeclared units

$$v_{15} = v2sub2prod\_compinhib (HXKfru\_g\_Vmax, HXKfru\_g\_Keq, [Fru\_g], HXKfru\_g\_KmFru, \\ [ATP\_g], HXKfru\_g\_KmATP, [Fru6P\_g], HXKfru\_g\_KmFru6P, [ADP\_g], \\ HXKfru\_g\_KmADP, [Glc\_g], HXKfru\_g\_KiGlc, [Glc6P\_g], HXKfru\_g\_KiGlc6P) \\ (49)$$

 $v2sub2prod\_compinhib \left(Vfmax, Keq, S1, Ks1, S2, Ks2, P1, Kp1, P2, Kp2, I1, Ki1, I2, Ki2\right)$ 

$$= \frac{V f max \cdot S1 \cdot S2 \cdot \left(1 - \frac{P1 \cdot P2}{Keq \cdot S1 \cdot S2}\right)}{Ks1 \cdot Ks2 \cdot \left(1 + \frac{S1}{Ks1} + \frac{P1}{Kp1}\right) \cdot \left(1 + \frac{S2}{Ks2} + \frac{P2}{Kp2} + \frac{I1}{Ki1} + \frac{I2}{Ki2}\right)}$$
(50)

Table 64: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
HXKfru_g- _Vmax	HXKfru_g_Vmax		1774.680		Ø
HXKfru_g_Keq HXKfru_g- _KmFru	HXKfru_g_Keq HXKfru_g_KmFru		631.000 0.350		<b>✓</b>
HXKfru_g- _KmATP	HXKfru_g- _KmATP		0.116		
HXKfru_g- _KmFru6P	HXKfru_g- _KmFru6P		2.700		

Id	Name	SBO	Value	Unit	Constant
HXKfru_g- _KmADP	HXKfru_g- KmADP		0.126		$\square$
HXKfru_g- _KiGlc	HXKfru_g_KiGlc		0.100		$\mathbf{Z}$
HXKfru_g- _KiGlc6P	HXKfru_g- _KiGlc6P		2.700		$\square$

# 6.16 Reaction G6PP\_c

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

Name G6PP\_c

# **Reaction equation**

$$Glc6P_c \xrightarrow{Glc6P_c, Glc_c} Glc_c$$
 (51)

#### Reactant

Table 65: Properties of each reactant.

Id	Name	SBO
Glc6P_c	Glc6P_c	

#### **Modifiers**

Table 66: Properties of each modifier.

Id	Name	SBO
Glc6P_c Glc_c	Glc6P_c Glc_c	

# **Product**

Table 67: Properties of each product.

Id	Name	SBO
Glc_c	Glc_c	

#### **Derived unit** contains undeclared units

$$v_{16} = v1sub1prod (G6PP\_c\_Vmax, G6PP\_c\_Keq, [Glc6P\_c], G6PP\_c\_KmGlc6P, [Glc\_c], G6PP\_c\_KmGlc)$$

$$(52)$$

$$v1sub1prod\left(Vfmax, Keq, S, Ks, P, Kp\right) = \frac{Vfmax \cdot S \cdot \left(1 - \frac{P}{Keq \cdot S}\right)}{Ks \cdot \left(1 + \frac{S}{Ks} + \frac{P}{Kp}\right)}$$
 (53)

Table 68: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
G6PP_c_Vmax	G6PP_c_Vmax		28.0		$ \mathbf{Z} $
$G6PP\_c\_Keq$	G6PP_c_Keq		263.0		
G6PP_c-	G6PP_c_KmGlc6P		5.6		$\square$
$_{\tt KmGlc6P}$					
${\tt G6PP\_c\_KmGlc}$	$G6PP\_c\_KmGlc$		5.6		

## 6.17 Reaction AK\_c

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

#### Name AK\_c

#### **Reaction equation**

$$2 ADP_{-c} \xrightarrow{ADP_{-c}, AMP_{-c}, ATP_{-c}} AMP_{-c} + ATP_{-c}$$
(54)

#### 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	
$\mathtt{AMP}_\mathtt{c}$	$AMP_c$	
$\mathtt{ATP}_\mathtt{c}$	ATP_c	

## **Products**

Table 71: Properties of each product.

Id	Name	SBO
AMP_c	AMP_c	
$\mathtt{ATP}_{-}\mathtt{c}$	ATP_c	

#### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{17} = vAK([ADP_c], [AMP_c], [ATP_c], AK_c_k1, AK_c_k2)$$
 (55)

$$vAK(ADP,AMP,ATP,k1,k2) = k1 \cdot ADP^2 - AMP \cdot ATP \cdot k2$$
 (56)

Table 72: 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	

## **6.18 Reaction PGI\_g**

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

Name PGI\_g

## **Reaction equation**

$$Glc6P\_g \xrightarrow{-6PG\_g, Glc6P\_g, Fru6P\_g, \_6PG\_g} Fru6P\_g$$
 Fru6P\\_g (57)

## Reactant

Table 73: Properties of each reactant.

Id	Name	SBO
Glc6P_g	Glc6P_g	

## **Modifiers**

Table 74: Properties of each modifier.

Id	Name	SBO
_6PG_g	_6PG_g	
${\tt Glc6P\_g}$	Glc6P_g	
$Fru6P_g$	Fru6P_g	
_6PG_g	_6PG_g	

#### **Product**

Table 75: Properties of each product.

Id	Name	SBO
Fru6P_g	Fru6P_g	

#### **Kinetic Law**

$$v_{18} = \frac{PGI\_g\_Vmax \cdot [Glc6P\_g] \cdot \left(1 - \frac{[Fru6P\_g]}{PGI\_g\_Keq \cdot [Glc6P\_g]}\right)}{PGI\_g\_KmGlc6P \cdot \left(1 + \frac{[Glc6P\_g]}{PGI\_g\_KmGlc6P} + \frac{[Fru6P\_g]}{PGI\_g\_KmFru6P} + \frac{[\_6PG\_g]}{PGI\_g\_Ki6PG}\right)}$$
(58)

Table 76: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
PGI_g_Vmax	PGI_g_Vmax		1305.000		$\overline{Z}$
PGI_g-	PGI_g_KmGlc6P		0.400		$\mathbf{Z}$
$_{\tt L}{\tt KmGlc6P}$					
$PGI_g_Keq$	PGI_g_Keq		0.457		
PGI_g-	PGI_g_KmFru6P		0.120		$   \overline{\mathbf{Z}} $
_KmFru6P					
$PGI_g_Ki6PG$	PGI_g_Ki6PG		0.140		

## 6.19 Reaction HXKfru\_c

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

Name HXKfru\_c

## **Reaction equation**

$$Fru\_c + ATP\_c \xrightarrow{Glc\_c, Glc6P\_c, Fru\_c, ATP\_c, Fru6P\_c, ADP\_c, Glc\_c, Glc6P\_c} ADP\_c + Fru6P\_c$$

$$(59)$$

## **Reactants**

Table 77: Properties of each reactant.

Id	Name	SBO
Fru_c	Fru_c	
$ATP_c$	ATP_c	

#### **Modifiers**

Table 78: Properties of each modifier.

Id	Name	SBO
Glc_c	Glc_c	
${\tt Glc6P\_c}$	Glc6P_c	
$Fru\_c$	Fru_c	
$ATP_c$	ATP_c	
$Fru6P_c$	Fru6P_c	
$ADP_c$	$ADP_c$	
${\tt Glc\_c}$	$Glc_c$	
Glc6P_c	Glc6P_c	

## **Products**

Table 79: Properties of each product.

Id	Name	SBO
ADP_c	ADP_c	
$Fru6P_c$	Fru6P_c	

#### **Kinetic Law**

#### **Derived unit** contains undeclared units

 $v_{19} = v2sub2prod\_compinhib (HXKfru\_c\_Vmax, HXKfru\_c\_Keq, [Fru\_c], HXKfru\_c\_KmFru, \\ [ATP\_c], HXKfru\_c\_KmATP, [Fru6P\_c], HXKfru\_c\_KmFru6P, [ADP\_c], \\ HXKfru\_c\_KmADP, [Glc\_c], HXKfru\_c\_KiGlc, [Glc6P\_c], HXKfru\_c\_KiGlc6P) \\ (60)$ 

v2sub2prod\_compinhib (Vfmax, Keq, S1, Ks1, S2, Ks2, P1, Kp1, P2, Kp2, I1, Ki1, I2, Ki2)

$$= \frac{V f max \cdot S1 \cdot S2 \cdot \left(1 - \frac{P1 \cdot P2}{Keq \cdot S1 \cdot S2}\right)}{Ks1 \cdot Ks2 \cdot \left(1 + \frac{S1}{Ks1} + \frac{P1}{Kp1}\right) \cdot \left(1 + \frac{S2}{Ks2} + \frac{P2}{Kp2} + \frac{I1}{Ki1} + \frac{I2}{Ki2}\right)}$$
(61)

Table 80: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
HXKfru_c-	HXKfru_c_Vmax		154.320		Ø
$_{ t Vmax}$					
${\tt HXKfru\_c\_Keq}$	HXKfru_c_Keq		631.000		
HXKfru_c-	HXKfru_c_KmFru		0.350		
$_{ m L}$ Km ${ t Fru}$					
HXKfru_c-	HXKfru_c_KmATP		0.116		
_KmATP					
HXKfru_c-	HXKfru_c-		2.700		
_KmFru6P	_KmFru6P				
HXKfru_c-	HXKfru_c-		0.126		
_KmADP	_KmADP				
HXKfru_c-	HXKfru_c_KiGlc		0.100		
$_{ extsf{KiGlc}}$					
HXKfru_c-	HXKfru_c-		2.700		
_KiGlc6P	_KiGlc6P				

## 6.20 Reaction TOX\_c

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

# **Reaction equation**

Name TOX\_c

$$TSH2\_c \xrightarrow{TSH2\_c} TS2\_c$$
 (62)

#### Reactant

Table 81: Properties of each reactant.

Id	Name	SBO
TSH2_c	TSH2_c	

## **Modifier**

Table 82: Properties of each modifier.

Id	Name	SBO
TSH2_c	TSH2_c	

## **Product**

Table 83: Properties of each product.

Id	Name	SBO
TS2_c	TS2_c	

## **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{20} = \text{mass\_action\_irrev} (\text{TOX\_c\_k}, [\text{TSH2\_c}])$$
 (63)

$$mass\_action\_irrev(k, S) = k \cdot S$$
 (64)

Table 84: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
TOX_c_k	TOX_c_k	2.0	

# 6.21 Reaction GDA\_g

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

## Name $GDA_g$

## **Reaction equation**

$$Gly3P\_g + DHAP\_c \xleftarrow{Gly3P\_g, \ DHAP\_c, \ Gly3P\_c, \ DHAP\_g} Gly3P\_c + DHAP\_g \tag{65}$$

## **Reactants**

Table 85: Properties of each reactant.

Id	Name	SBO
Gly3P_g DHAP_c	Gly3P_g 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	

#### **Products**

Table 87: Properties of each product.

Id	Name	SBO
Gly3P_c DHAP_g	Gly3P_c DHAP_g	

## **Kinetic Law**

$$v_{21} = [Gly3P\_g] \cdot GDA\_g\_k \cdot [DHAP\_c] - [Gly3P\_c] \cdot GDA\_g\_k \cdot [DHAP\_g]$$
 (66)

Table 88: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
GDA_g_k	GDA_g_k	600.0	

## **6.22 Reaction** FruT\_g

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

Name FruT\_g

## **Reaction equation**

$$Fru\_c \xrightarrow{Fru\_c, Fru\_g} Fru\_g$$
 (67)

#### Reactant

Table 89: Properties of each reactant.

Id	Name	SBO
Fru_c	Fru_c	

#### **Modifiers**

Table 90: Properties of each modifier.

Id	Name	SBO
Fru_c	Fru_c	
Fru_g	Fru_g	

## **Product**

Table 91: Properties of each product.

Id	Name	SBO
Fru_g	Fru_g	

## **Kinetic Law**

$$v_{22} = \text{mass\_action\_rev} (\text{FruT\_g\_k1}, [\text{Fru\_c}], \text{FruT\_g\_k2}, [\text{Fru\_g}])$$
(68)

$$mass\_action\_rev(k1, S, k2, P) = k1 \cdot S - k2 \cdot P$$
 (69)

Table 92: Properties of each parameter.

Id	Name	SBO Value	e Unit	Constant
FruT_g_k1	FruT_g_k1	250000	0.0	
$FruT_g_k2$	FruT_g_k2	250000	0.0	$\mathbf{Z}$

## 6.23 Reaction PGL\_c

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

## Name PGL\_c

## **Reaction equation**

$$_{6}PGL_{c} \stackrel{\underline{-6}PGL_{c}, \underline{-6}PG\underline{c}}{\longleftarrow} _{6}PG_{c}$$
 (70)

#### Reactant

Table 93: Properties of each reactant.

Id	Name	SBO
_6PGL_c	_6PGL_c	

#### **Modifiers**

Table 94: Properties of each modifier.

Id	Name	SBO
_6PGL_c _6PG_c	_6PGL_c _6PG_c	

#### **Product**

Table 95: Properties of each product.

Id	Name	SBO
_6PG_c	_6PG_c	

#### **Kinetic Law**

$$v_{23} = PGL\_c\_k \cdot vol\left(cytosol\right) \cdot \left(\left[\_6PGL\_c\right] - \frac{\left[\_6PG\_c\right]}{PGL\_c\_Keq}\right) + v1sub1prod\left(PGL\_c\_Vmax, \quad (71)\right) \\ PGL\_c\_Keq, \left[\_6PGL\_c\right], PGL\_c\_Km6PGL, \left[\_6PG\_c\right], PGL\_c\_Km6PG)$$

$$v1sub1prod\left(Vfmax,Keq,S,Ks,P,Kp\right) = \frac{Vfmax \cdot S \cdot \left(1 - \frac{P}{Keq \cdot S}\right)}{Ks \cdot \left(1 + \frac{S}{Ks} + \frac{P}{Kp}\right)} \tag{72}$$

$$v1sub1prod\left(Vfmax,Keq,S,Ks,P,Kp\right) = \frac{Vfmax \cdot S \cdot \left(1 - \frac{P}{Keq \cdot S}\right)}{Ks \cdot \left(1 + \frac{S}{Ks} + \frac{P}{Kp}\right)} \tag{73}$$

Table 96: 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		$   \overline{\mathscr{L}} $

## 6.24 Reaction FruT\_c

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

Name FruT\_c

## **Reaction equation**

$$Fru_e \xrightarrow{Fru_e, Fru_c} Fru_c \tag{74}$$

#### Reactant

Table 97: Properties of each reactant.

Id	Name	SBO
Fru_e	Fru_e	

#### **Modifiers**

Table 98: Properties of each modifier.

Id	Name	SBO
Fru_e	Fru_e	
$Fru_c$	Fru_c	

#### **Product**

Table 99: Properties of each product.

Id	Name	SBO
Fru_c	Fru_c	

#### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{24} = \frac{\text{FruT\_c\_Vmax} \cdot ([\text{Fru\_e}] - [\text{Fru\_c}])}{\text{FruT\_c\_KmFru} + [\text{Fru\_e}] + [\text{Fru\_c}] + \frac{\text{FruT\_c\_alpha} \cdot [\text{Fru\_e}] \cdot [\text{Fru\_c}]}{\text{FruT\_c\_KmFru}}}$$
(75)

Table 100: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
FruT_c_Vmax	FruT_c_Vmax		69.10		
FruT_c_KmFru	FruT_c_KmFru		3.91		
FruT_c_alpha	FruT_c_alpha		0.75		<b>✓</b>

# 6.25 Reaction AK\_g

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

Name  $AK_{-}g$ 

## **Reaction equation**

$$2 ADP_{-g} \xrightarrow{ADP_{-g}, AMP_{-g}, ATP_{-g}} AMP_{-g} + ATP_{-g}$$
(76)

#### Reactant

Table 101: Properties of each reactant.

Id	Name	SBO
ADP_g	ADP_g	

## **Modifiers**

Table 102: Properties of each modifier.

Id	Name	SBO
ADP_g AMP_g ATP_g	ADP_g AMP_g ATP_g	

#### **Products**

Table 103: Properties of each product.

Id	Name	SBO
$AMP_g$	$AMP_{-}g$	
$\mathtt{ATP}_{-}\mathtt{g}$	$ATP_{-}g$	

## **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{25} = vAK([ADP_g], [AMP_g], [ATP_g], AK_g_k1, AK_g_k2)$$
 (77)

$$vAK(ADP,AMP,ATP,k1,k2) = k1 \cdot ADP^2 - AMP \cdot ATP \cdot k2$$
 (78)

Table 104: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
AK_g_k1	$AK_g_k1$	480.0	Ø
$AK_g_k2$	$AK_g_k2$	1000.0	

## **6.26 Reaction** \_6PGDH\_c

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

## Name \_6PGDH\_c

## **Reaction equation**

$$NADP\_c + \_6PG\_c \xrightarrow{\_6PG\_c, \ NADP\_c, \ Rul5P\_c, \ NADPH\_c} CO2\_c + NADPH\_c + Rul5P\_c \tag{79}$$

#### **Reactants**

Table 105: Properties of each reactant.

Id	Name	SBO
NADP_c	NADP_c	
_6PG_c	_6PG_c	

#### **Modifiers**

Table 106: 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 107: Properties of each product.

Id	Name	SBO
CO2_c	CO2_c	
$NADPH_c$	NADPH_c	
$Rul5P_c$	Rul5P_c	

#### **Kinetic Law**

$$v_{26} = v_{2}sub_{2}prod(_{6}PGDH_{c}Vmax, _{6}PGDH_{c}Keq, [_{6}PG_{c}], _{6}PGDH_{c}Km6PG, \\ [NADP_{c}], _{6}PGDH_{c}KmNADP, [Rul5P_{c}], _{6}PGDH_{c}KmRul5P, [NADPH_{c}], \\ [80] \\ \_{6}PGDH_{c}KmNADPH)$$

$$\begin{aligned} &v2sub2prod\left(Vfmax, Keq, S1, Ks1, S2, Ks2, P1, Kp1, P2, Kp2\right) \\ &= \frac{Vfmax \cdot S1 \cdot S2 \cdot \left(1 - \frac{P1 \cdot P2}{Keq \cdot S1 \cdot S2}\right)}{Ks1 \cdot Ks2 \cdot \left(1 + \frac{S1}{Ks1} + \frac{P1}{Kp1}\right) \cdot \left(1 + \frac{S2}{Ks2} + \frac{P2}{Kp2}\right)} \end{aligned} \tag{81}$$

Table 108: 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		$\overline{\mathbf{Z}}$
_6PGDH_c-	_6PGDH_c-		0.004		$\overline{\mathbf{Z}}$
_Km6PG	_Km6PG				
_6PGDH_c-	_6PGDH_c-		0.001		
_KmNADP	_KmNADP				
_6PGDH_c-	_6PGDH_c-		0.030		
_KmRul5P	_KmRul5P				
_6PGDH_c-	_6PGDH_c-		$6 \cdot 10^{-4}$		
_KmNADPH	_KmNADPH				_

## 6.27 Reaction PPI\_c

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

## Name $PPI\_c$

## **Reaction equation**

$$Rul5P_c \xrightarrow{Rul5P_c, Rib5P_c} Rib5P_c$$
 (82)

#### Reactant

Table 109: Properties of each reactant.

Id	Name	SBO
Rul5P_c	Rul5P_c	

## **Modifiers**

Table 110: Properties of each modifier.

Id	Name	SBO
Rul5P_c		
$Rib5P_c$	Rib5P_c	

## **Product**

Table 111: Properties of each product.

Id	Name	SBO
Rib5P_c	Rib5P_c	

## **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{27} = v1sub1prod(PPI\_c\_Vmax, PPI\_c\_Keq, [Rul5P\_c], PPI\_c\_KmRul5P, [Rib5P\_c], PPI\_c\_KmRib5P)$$

$$(83)$$

$$v1sub1prod\left(Vfmax,Keq,S,Ks,P,Kp\right) = \frac{Vfmax \cdot S \cdot \left(1 - \frac{P}{Keq \cdot S}\right)}{Ks \cdot \left(1 + \frac{S}{Ks} + \frac{P}{Kp}\right)} \tag{84}$$

Table 112: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
PPI_c_Vmax PPI_c_Keq	PPI_c_Vmax PPI_c_Keq	72.0 5.6	<b>Ø</b>
PPI_c- _KmRu15P	PPI_c_KmRul5P	1.4	
PPI_c- _KmRib5P	PPI_c_KmRib5P	4.0	

# **6.28 Reaction PPI\_g**

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

Name PPI\_g

## **Reaction equation**

$$Rul5P\_g \xrightarrow{Rul5P\_g, Rib5P\_g} Rib5P\_g$$
 (85)

#### Reactant

Table 113: Properties of each reactant.

Id	Name	SBO
Rul5P_g	Rul5P_g	

#### **Modifiers**

Table 114: Properties of each modifier.

Id	Name	SBO
Rul5P_g	Rul5P_g	
Rib5P_g	Rib5P_g	

#### **Product**

Table 115: Properties of each product.

Id	Name	SBO
Rib5P_g	Rib5P_g	

## **Kinetic Law**

$$\begin{array}{l} \textit{v}_{28} = \textit{v}1\textit{sub}1\textit{prod}\left(\textit{PPI\_g\_Vmax}, \textit{PPI\_g\_Keq}, [\textit{Rul5P\_g}], \textit{PPI\_g\_KmRul5P}, [\textit{Rib5P\_g}], \\ \textit{PPI\_g\_KmRib5P} \end{array} \right) \tag{86}$$

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

Table 116: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
PPI_g_Vmax PPI_g_Keq PPI_g-	PPI_g_Vmax PPI_g_Keq PPI_g_KmRul5P		72.0 5.6 1.4		<b>I</b> <b>I</b> <b>I</b>
_KmRu15P PPI_g- _KmRib5P	PPI_g_KmRib5P		4.0		

## 6.29 Reaction \_6PGDH\_g

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

Name \_6PGDH\_g

## **Reaction equation**

$$\_6PG\_g + NADP\_g \xleftarrow{\_6PG\_g, \ NADP\_g, \ Rul5P\_g, \ NADPH\_g} Rul5P\_g + CO2\_g + NADPH\_g \tag{88}$$

## **Reactants**

Table 117: Properties of each reactant.

Id	Name	SBO
_6PG_g	_6PG_g	
$NADP_g$	$NADP_{-}g$	

## **Modifiers**

Table 118: 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 119: Properties of each product.

Id	Name	SBO
Rul5P_g CO2_g NADPH_g	Rul5P_g CO2_g NADPH_g	

## **Kinetic Law**

Derived unit contains undeclared units

$$v_{29} = v_2sub_2prod(\_6PGDH\_g\_Vmax, \_6PGDH\_g\_Keq, [\_6PG\_g], \_6PGDH\_g\_Km6PG, \\ [NADP\_g], \_6PGDH\_g\_KmNADP, [Rul5P\_g], \_6PGDH\_g\_KmRul5P,$$

$$[NADPH\_g], \_6PGDH\_g\_KmNADPH)$$

$$[NADPH\_g], \_6PGDH\_g\_KmNADPH)$$

$$v2sub2prod (Vfmax, Keq, S1, Ks1, S2, Ks2, P1, Kp1, P2, Kp2)$$

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

$$(90)$$

Table 120: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
_6PGDH_g_Vmax	_6PGDH_g_Vmax		10.600		$\overline{Z}$
_6PGDH_g_Keq	_6PGDH_g_Keq		47.000		$\overline{\checkmark}$
_6PGDH_g-	_6PGDH_g-		0.004		
_Km6PG	_Km6PG				
_6PGDH_g-	_6PGDH_g-		0.001		
_KmNADP	_KmNADP				
_6PGDH_g-	_6PGDH_g-		0.030		$\square$
_KmRul5P	_KmRul5P				
_6PGDH_g-	_6PGDH_g-		$6 \cdot 10^{-4}$		
_KmNADPH	_KmNADPH				

## 6.30 Reaction GlcT\_g

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

Name GlcT\_g

## **Reaction equation**

$$Glc\_c \xrightarrow{Glc\_c, Glc\_g} Glc\_g$$
 (91)

## Reactant

Table 121: Properties of each reactant.

Id	Name	SBO
Glc_c	Glc_c	

## **Modifiers**

Table 122: Properties of each modifier.

Id	Name	SBO
Glc_c	Glc_c	
Glc_g	Glc_g	

## **Product**

Table 123: Properties of each product.

Id	Name	SBO
Glc_g	Glc_g	

## **Kinetic Law**

$$v_{30} = \text{mass\_action\_rev} \left( \text{GlcT\_g\_k1}, [\text{Glc\_c}], \text{GlcT\_g\_k2}, [\text{Glc\_g}] \right)$$
 (92)

mass\_action\_rev 
$$(k1, S, k2, P) = k1 \cdot S - k2 \cdot P$$
 (93)

Table 124: 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	$\square$

## 6.31 Reaction GlcT\_c

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

Name GlcT\_c

## **Reaction equation**

$$Glc_e \xrightarrow{Glc_e, Glc_c} Glc_c$$
 (94)

#### Reactant

Table 125: Properties of each reactant.

Id	Name	SBO
Glc_e	Glc_e	

#### **Modifiers**

Table 126: Properties of each modifier.

Id	Name	SBO
Glc_e	Glc_e	
${\tt Glc\_c}$	Glc_c	

## **Product**

Table 127: Properties of each product.

Id	Name	SBO
Glc_c	$Glc\_c$	

## **Kinetic Law**

$$v_{31} = \frac{\text{GlcT\_c\_Vmax} \cdot ([\text{Glc\_e}] - [\text{Glc\_c}])}{\text{GlcT\_c\_KmGlc} + [\text{Glc\_e}] + [\text{Glc\_c}] + \frac{\text{GlcT\_c\_alpha\cdot[Glc\_e]\cdot[Glc\_c]}}{\text{GlcT\_c\_KmGlc}}}$$
(95)

Table 128: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
${\tt GlcT\_c\_Vmax}$	GlcT_c_Vmax		111.70		
${\tt GlcT\_c\_KmGlc}$	GlcT_c_KmGlc		1.00		
${ t GlcT_c_alpha}$	GlcT_c_alpha		0.75		

## **6.32 Reaction PGL\_g**

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

Name  $PGL_g$ 

## **Reaction equation**

$$\_6PGL\_g \xrightarrow{\_6PGL\_g, \_6PG\_g} \_6PG\_g$$
 (96)

#### Reactant

Table 129: Properties of each reactant.

Id	Name	SBO
_6PGL_g	_6PGL_g	

## **Modifiers**

Table 130: Properties of each modifier.

Id	Name	SBO
_6PGL_g	_6PGL_g	
_6PG_g	_6PG_g	

## **Product**

Table 131: Properties of each product.

Id	Name	SBO
_6PG_g	_6PG_g	

#### **Kinetic Law**

#### **Derived unit** contains undeclared units

$$\begin{aligned} v_{32} &= vol\left(glycosome\right) \cdot PGL\_g\_k \cdot \left(\left[\_6PGL\_g\right] - \frac{\left[\_6PG\_g\right]}{PGL\_g\_Keq}\right) + v1sub1prod\left(PGL\_g\_Vmax, \\ &PGL\_g\_Keq,\left[\_6PGL\_g\right], PGL\_g\_Km6PGL,\left[\_6PG\_g\right], PGL\_g\_Km6PG\right) \end{aligned} \tag{97}$$

$$v1sub1prod\left(Vfmax,Keq,S,Ks,P,Kp\right) = \frac{Vfmax \cdot S \cdot \left(1 - \frac{P}{Keq \cdot S}\right)}{Ks \cdot \left(1 + \frac{S}{Ks} + \frac{P}{Kp}\right)} \tag{98}$$

$$v1sub1prod\left(Vfmax, Keq, S, Ks, P, Kp\right) = \frac{Vfmax \cdot S \cdot \left(1 - \frac{P}{Keq \cdot S}\right)}{Ks \cdot \left(1 + \frac{S}{Ks} + \frac{P}{Kp}\right)} \tag{99}$$

Table 132: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
PGL_g_Vmax	PGL_g_Vmax		5.000		Ø
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		$\checkmark$

#### 6.33 Reaction TR\_c

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

## Name TR\_c

## **Reaction equation**

$$TS2\_c + NADPH\_c \xrightarrow{TS2\_c, NADPH\_c, TSH2\_c, NADP\_c} NADP\_c + TSH2\_c$$
 (100)

#### Reactants

Table 133: Properties of each reactant.

Id	Name	SBO
TS2_c	TS2_c	
$NADPH_c$	NADPH_c	

## **Modifiers**

Table 134: 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 135: Properties of each product.

Id	Name	SBO
NADP_c	NADP_c	
TSH2_c	TSH2_c	

#### **Kinetic Law**

$$v_{33} = v2sub2prod(TR\_c\_Vmax, TR\_c\_Keq, [TS2\_c], TR\_c\_KmTS2, [NADPH\_c], TR\_c\_KmNADPH, [TSH2\_c], TR\_c\_KmTSH2, [NADP\_c], TR\_c\_KmNADP)$$

$$(101)$$

$$= \frac{V \text{fmax} \cdot \text{S1} \cdot \text{S2} \cdot \left(1 - \frac{P1 \cdot P2}{\text{Keq} \cdot \text{S1} \cdot \text{S2}}\right)}{\text{Ks1} \cdot \text{Ks2} \cdot \left(1 + \frac{S1}{\text{Ks1}} + \frac{P1}{\text{Kp1}}\right) \cdot \left(1 + \frac{S2}{\text{Ks2}} + \frac{P2}{\text{Kp2}}\right)}$$
(102)

Table 136: 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		
$TR_c_{KmNADPH}$	$TR_c_KmNADPH$		$7.7\cdot10^{-4}$		
$TR_c_KmTSH2$	$TR_c_KmTSH2$		0.002		
$TR_c_KmNADP$	$TR_c_KmNADP$		0.081		

# **6.34 Reaction PGK\_g**

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

## Name $PGK_{-}g$

## **Reaction equation**

$$\_13BPGA\_g + ADP\_g \xrightarrow{-13BPGA\_g, \ ADP\_g, \ \_3PGA\_g, \ ATP\_g} \_3PGA\_g + ATP\_g \qquad (103)$$

## **Reactants**

Table 137: Properties of each reactant.

Id	Name	SBO
_13BPGA_g	_13BPGA_g	
$ADP_g$	$ADP_{-}g$	

## **Modifiers**

Table 138: Properties of each modifier.

Id	Name	SBO
_13BPGA_g	_13BPGA_g	
$\mathtt{ADP}_{-}\mathtt{g}$	$ADP_{-}g$	
_3PGA_g	_3PGA_g	
ATP_g	ATP_g	

## **Products**

Table 139: Properties of each product.

Id	Name	SBO
_3PGA_g	_3PGA_g	
ATP_g	$ATP_{-}g$	

#### **Kinetic Law**

#### **Derived unit** contains undeclared units

$$v_{34} = v2sub2prod(PGK\_g\_Vmax, PGK\_g\_Keq, [\_13BPGA\_g], PGK\_g\_Km13BPGA, [ADP\_g], \\ PGK\_g\_KmADP, [\_3PGA\_g], PGK\_g\_Km3PGA, [ATP\_g], PGK\_g\_KmATP) \\ (104)$$

$$v2sub2prod (Vfmax, Keq, S1, Ks1, S2, Ks2, P1, Kp1, P2, Kp2)$$

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

$$(105)$$

Table 140: Properties of each parameter.

Tuble 110.11oporties of each parameter.					
Id	Name	SBO	Value	Unit	Constant
PGK_g_Vmax	PGK_g_Vmax		2862.000		$ \mathbf{Z} $
PGK_g_Keq	PGK_g_Keq		3377.000		$\mathbf{Z}$
PGK_g-	PGK_g-		0.003		$\mathbf{Z}$
_Km13BPGA	_Km13BPGA				
$PGK\_g\_KmADP$	$PGK_g_KmADP$		0.100		
$PGK_g_Km3PGA$	PGK_g_Km3PGA		1.620		
PGK_g_KmATP	$PGK_g_KmATP$		0.290		

## 6.35 Reaction G3PDH\_g

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

## Name G3PDH\_g

## **Reaction equation**

$$NADH_{-}g + DHAP_{-}g \xrightarrow{DHAP_{-}g, \ NADH_{-}g, \ Gly3P_{-}g, \ NAD_{-}g} Gly3P_{-}g + NAD_{-}g \qquad (106)$$

#### **Reactants**

Table 141: Properties of each reactant.

Id	Name	SBO
NADH_g	NADH_g	
$\mathtt{DHAP}_{\mathtt{g}}$	DHAP_g	

#### **Modifiers**

Table 142: Properties of each modifier.

Id	Name	SBO
DHAP_g	DHAP_g	
$NADH_g$	$NADH_{-}g$	
${\tt Gly3P\_g}$	Gly3P_g	
$NAD_g$	$NAD_{-}g$	

#### **Products**

Table 143: Properties of each product.

Id	Name	SBO
Gly3P_g	Gly3P_g	
$NAD_g$	$NAD_{-}g$	

#### **Kinetic Law**

$$v_{35} = v_2 sub_2 prod (G3PDH_g_Vmax, G3PDH_g_Keq, [DHAP_g], G3PDH_g_KmDHAP, \\ [NADH_g], G3PDH_g_KmNADH, [Gly3P_g], G3PDH_g_KmGly3P, [NAD_g], \\ G3PDH_g_KmNAD)$$

$$\begin{split} v2sub2prod \left(Vfmax, Keq, S1, Ks1, S2, Ks2, P1, Kp1, P2, Kp2\right) \\ &= \frac{Vfmax \cdot S1 \cdot S2 \cdot \left(1 - \frac{P1 \cdot P2}{Keq \cdot S1 \cdot S2}\right)}{Ks1 \cdot Ks2 \cdot \left(1 + \frac{S1}{Ks1} + \frac{P1}{Kp1}\right) \cdot \left(1 + \frac{S2}{Ks2} + \frac{P2}{Kp2}\right)} \end{split} \tag{108}$$

Table 144: 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		$   \overline{\mathscr{A}} $
G3PDH_g-	G3PDH_g-		0.10		$   \overline{\mathscr{A}} $
_KmDHAP	_KmDHAP				
G3PDH_g-	G3PDH_g-		0.01		$\square$
$_{ m L}$ KmNADH	_KmNADH				
G3PDH_g-	G3PDH_g-		2.00		
$_{ t KmGly3P}$	_KmGly3P				
G3PDH_g-	G3PDH_g-		0.40		
_KmNAD	_KmNAD				

## 6.36 Reaction ATPu\_c

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

Name ATPu\_c

## **Reaction equation**

$$ATP_{-}c \xrightarrow{ATP_{-}c, ADP_{-}c} ADP_{-}c$$
 (109)

## Reactant

Table 145: Properties of each reactant.

Id	Name	SBO
ATP_c	ATP_c	

#### **Modifiers**

Table 146: Properties of each modifier.

Id	Name	SBO
ATP_c	ATP_c	
$ADP_c$	$ADP_c$	

## **Product**

Table 147: Properties of each product.

Id	Name	SBO
ADP_c	ADP_c	

#### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{36} = \frac{\text{ATPu\_c\_k} \cdot [\text{ATP\_c}]}{[\text{ADP\_c}]}$$
 (110)

Table 148: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
ATPu_c_k	ATPu_c_k	50.0	

## 6.37 Reaction GK\_g

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

## Name GK\_g

## **Reaction equation**

$$Gly3P\_g + ADP\_g \xrightarrow{Gly3P\_g, ADP\_g, Gly\_e, ATP\_g} Gly\_e + ATP\_g$$
 (111)

#### **Reactants**

Table 149: Properties of each reactant.

Id	Name	SBO
Gly3P_g ADP_g	Gly3P_g ADP_g	

## **Modifiers**

Table 150: Properties of each modifier.

Id	Name	SBO
Gly3P_g	Gly3P_g	

Id	Name	SBO
ADP_g Gly_e ATP_g	ADP_g Gly_e ATP_g	

#### **Products**

Table 151: Properties of each product.

Id	Name	SBO
J	Gly_e	
AIP_g	ATP_g	

## **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{37} = v2sub2prod(GK\_g\_Vmax, GK\_g\_Keq, [Gly3P\_g], GK\_g\_KmGly3P, [ADP\_g], GK\_g\_KmADP, [Gly\_e], GK\_g\_KmGly, [ATP\_g], GK\_g\_KmATP)$$
 (112)

$$v2sub2prod (Vfmax, Keq, S1, Ks1, S2, Ks2, P1, Kp1, P2, Kp2)$$

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

$$(113)$$

Table 152: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
$GK_g_Vmax$	GK_g_Vmax		200.000		Ø
$GK_g_Keq$	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		

## 6.38 Reaction ALD\_g

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

## Name ALD\_g

## **Reaction equation**

$$Fru16BP\_g \xrightarrow{ATP\_g, ADP\_g, AMP\_g, Fru16BP\_g, GA3P\_g, DHAP\_g, ATP\_g, ADP\_g, AMP\_g} GA3P\_g + DHAP\_g \tag{114}$$

## Reactant

Table 153: Properties of each reactant.

Id	Name	SBO
Fru16BP_g	Fru16BP_g	

#### **Modifiers**

Table 154: Properties of each modifier.

Id	Name	SBO
ATP_g	ATP_g	
$\mathtt{ADP}_{-}\mathtt{g}$	$ADP_{-}g$	
$\mathtt{AMP}_{-}\mathtt{g}$	$AMP_{-}g$	
Fru16BP_g	Fru16BP_g	
GA3P_g	GA3P_g	
$\mathtt{DHAP}_{\mathtt{g}}$	DHAP_g	
$\mathtt{ATP}_{-}\mathtt{g}$	$ATP_{-}g$	
$\mathtt{ADP}_{-}\mathtt{g}$	$ADP_{-}g$	
AMP_g	$AMP_{-}g$	

## **Products**

Table 155: Properties of each product.

Id	Name	SBO
GA3P_g	GA3P_g	
${\tt DHAP\_g}$	DHAP_g	

## **Kinetic Law**

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

ALD\_g\_V

Table 156: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
ALD_g_Vmax	ALD_g_Vmax		560.000		
ALD_g-	ALD_g-		0.009		$\overline{\mathbf{Z}}$
_KmFru16BP	_KmFru16BP				
ALD_g_KiATP	ALD_g_KiATP		0.680		$   \overline{\mathcal{L}} $
$ALD_g_KiADP$	ALD_g_KiADP		1.510		
$ALD_g_KiAMP$	ALD_g_KiAMP		3.650		
$\mathtt{ALD\_g\_Keq}$	ALD_g_Keq		0.084		
$\mathtt{ALD\_g\_KmGA3P}$	ALD_g_KmGA3P		0.067		
$\mathtt{ALD\_g\_KmDHAP}$	$ALD_{g}_{Km}DHAP$		0.015		$\square$
$ALD_g_KiGA3P$	ALD_g_KiGA3P		0.098		$\square$

## **6.39 Reaction GAPDH\_g**

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

#### Name GAPDH\_g

## **Reaction equation**

$$GA3P\_g + NAD\_g + Pi\_g \xrightarrow{GA3P\_g, NAD\_g, \_13BPGA\_g, NADH\_g} NADH\_g + \_13BPGA\_g$$

$$(116)$$

## **Reactants**

Table 157: Properties of each reactant.

Id	Name	SBO
$GA3P_g$	GA3P_g	
$NAD_{-}g$	$NAD_{-}g$	
Pi_g	Pi_g	

#### **Modifiers**

Table 158: Properties of each modifier.

Id	Name	SBO
GA3P_g	GA3P_g	
$\mathtt{NAD}_{\mathtt{g}}$	$NAD_{-}g$	
_13BPGA_g	_13BPGA_g	
$NADH_g$	NADH_g	

#### **Products**

Table 159: Properties of each product.

Id	Name	SBO
NADH_g _13BPGA_g	NADH_g _13BPGA_g	

#### **Kinetic Law**

$$v_{39} = v2sub2prod(GAPDH\_g\_Vmax,GAPDH\_g\_Keq,[GA3P\_g],GAPDH\_g\_KmGA3P,\\ [NAD\_g],GAPDH\_g\_KmNAD,[\_13BPGA\_g],GAPDH\_g\_Km13BPGA,[NADH\_g],\\ GAPDH\_g\_KmNADH)$$
 
$$(117)$$

$$v2sub2prod(Vfmax, Keq, S1, Ks1, S2, Ks2, P1, Kp1, P2, Kp2)$$

$$= \frac{Vfmax \cdot S1 \cdot S2 \cdot \left(1 - \frac{P1 \cdot P2}{Keq \cdot S1 \cdot S2}\right)}{Ks1 \cdot Ks2 \cdot \left(1 + \frac{S1}{Ks1} + \frac{P1}{Kp1}\right) \cdot \left(1 + \frac{S2}{Ks2} + \frac{P2}{Kp2}\right)}$$
(118)

Table 160: Properties of each parameter.

		1	1		
Id	Name	SBO	Value	Unit	Constant
GAPDH_g_Vmax	GAPDH_g_Vmax		720.900		$\square$
$GAPDH_g_Keq$	GAPDH_g_Keq		0.066		
GAPDH_g-	GAPDH_g-		0.150		
$_{\mathtt{KmGA3P}}$	_KmGA3P				
GAPDH_g-	GAPDH_g-		0.450		
$_{\tt KmNAD}$	_KmNAD				
GAPDH_g-	GAPDH_g-		0.100		
$_{\rm L}$ Km13BPGA	_Km13BPGA				

Id	Name	SBO	Value	Unit	Constant
GAPDH_g- _KmNADH	GAPDH_g- _KmNADH		0.020		Ø

## 6.40 Reaction GPO\_c

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

#### Name GPO\_c

## **Reaction equation**

$$Gly3P_c \xrightarrow{Gly3P_c} DHAP_c$$
 (119)

## Reactant

Table 161: Properties of each reactant.

Id	Name	SBO
Gly3P_c	Gly3P_c	

## **Modifier**

Table 162: Properties of each modifier.

Id	Name	SBO
Gly3P_c	Gly3P_c	

## **Product**

Table 163: Properties of each product.

Id	Name	SBO
DHAP_c	DHAP_c	

#### **Kinetic Law**

$$v_{40} = v1sub(GPO\_c\_Vmax, [Gly3P\_c], GPO\_c\_KmGly3P)$$
 (120)

$$v1sub\left(Vfmax,S,Ks\right) = \frac{Vfmax \cdot S}{Ks \cdot \left(1 + \frac{S}{Ks}\right)} \tag{121}$$

Table 164: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
GPO_c_Vmax GPO_cKmGly3P	GPO_c_Vmax GPO_c_KmGly3P		368.0 1.7		<b>Z</b>

# 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 Fru\_e

Name Fru\_e

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Fru}_{-}\mathrm{e} = 0 \tag{122}$$

## 7.2 Species \_2PGA\_c

Name \_2PGA\_c

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

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).

$$\frac{\mathrm{d}}{\mathrm{d}t} \cdot 2PGA \cdot c = |v_5| - |v_8| \tag{123}$$

## 7.3 Species Fru\_g

Name Fru\_g

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

This species takes part in six reactions (as a reactant in HXKfru\_g and as a product in FruT\_g and as a modifier in HXK\_g, HXK\_g, HXKfru\_g, FruT\_g).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Fru}_{-g} = |v_{22}| - |v_{15}| \tag{124}$$

## 7.4 Species Fru\_c

Name Fru\_c

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

This species takes part in eight reactions (as a reactant in HXKfru\_c, FruT\_g and as a product in FruT\_c and as a modifier in HXK\_c, HXKfru\_c, FruT\_g, FruT\_c).

$$\frac{d}{dt} Fru_{c} = v_{24} - v_{19} - v_{22}$$
 (125)

## 7.5 Species DHAP\_c

Name DHAP\_c

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

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).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{DHAP}_{-}c = v_{40} - v_{21} \tag{126}$$

## 7.6 Species ATP\_g

Name ATP\_g

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

This species takes part in 16 reactions (as a reactant in PFK\_g, HXK\_g, HXKfru\_g and as a product in RK\_g, AK\_g, PGK\_g, GK\_g and as a modifier in PFK\_g, HXK\_g, RK\_g, HXKfru\_g, AK\_g, PGK\_g, GK\_g, ALD\_g, ALD\_g).

$$\frac{d}{dt}ATP_{-}g = v_{10} + v_{25} + v_{34} + v_{37} - v_{3} - v_{9} - v_{15}$$
(127)

## 7.7 Species DHAP\_g

Name DHAP\_g

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

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).

$$\frac{d}{dt}DHAP_{g} = v_{21} + v_{38} - v_{1} - v_{35}$$
 (128)

## 7.8 Species ADP\_g

Name ADP\_g

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

This species takes part in 16 reactions (as a reactant in RK\_g, AK\_g, PGK\_g, GK\_g and as a product in PFK\_g, HXK\_g, HXKfru\_g and as a modifier in PFK\_g, HXK\_g, RK\_g, HXKfru\_g, AK\_g, PGK\_g, GK\_g, ALD\_g, ALD\_g).

$$\frac{d}{dt}ADP_{-g} = |v_3| + |v_9| + |v_{15}| - |v_{10}| - 2|v_{25}| - |v_{34}| - |v_{37}|$$
(129)

## 7.9 Species Glc6P\_g

Name Glc6P\_g

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

This species takes part in eight 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, HXKfru\_g, HXKfru\_g, PGI\_g).

$$\frac{d}{dt}Glc6P_{-g} = |v_9| - |v_4| - |v_{18}|$$
 (130)

## 7.10 Species ADP\_c

Name ADP\_c

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

This species takes part in ten reactions (as a reactant in PYK\_c, AK\_c and as a product in HXK\_c, HXKfru\_c, ATPu\_c and as a modifier in PYK\_c, HXK\_c, AK\_c, HXKfru\_c, ATPu\_c).

$$\frac{d}{dt}ADP_{c} = v_{13} + v_{19} + v_{36} - v_{2} - 2v_{17}$$
(131)

## 7.11 Species \_3PGA\_c

Name \_3PGA\_c

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

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).

$$\frac{d}{dt} - 3PGA_c = |v_{11}| - |v_5| \tag{132}$$

## 7.12 Species NADPH\_c

Name NADPH\_c

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

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).

$$\frac{d}{dt}NADPH_c = |v_7| + |v_{26}| - |v_{12}| - |v_{33}|$$
(133)

## 7.13 Species Fru6P\_g

Name Fru6P\_g

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

This species takes part in eight reactions (as a reactant in PFK\_g and as a product in HXKfru\_g, PGI\_g and as a modifier in PFK\_g, HXK\_g, HXK\_g, HXKfru\_g, PGI\_g).

$$\frac{d}{dt} Fru6P_{-g} = |v_{15}| + |v_{18}| - |v_{3}|$$
 (134)

#### 7.14 Species Fru6P\_c

Name Fru6P\_c

Initial concentration  $0.9 \text{ nmol} \cdot \mu l^{-1}$ 

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Fru6P}_{.c} = 0 \tag{135}$$

## 7.15 Species Pi\_g

Name Pi\_g

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

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:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Pi.g} = 0\tag{136}$$

## **7.16 Species** 02\_c

Name O2\_c

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{O}2_{-}\mathrm{c} = 0\tag{137}$$

## 7.17 Species NADP\_c

Name NADP\_c

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

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).

$$\frac{d}{dt}NADP_{c}c = |v_{12}| + |v_{33}| - |v_{7}| - |v_{26}|$$
(138)

## 7.18 Species ATP\_c

Name ATP\_c

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

This species takes part in ten reactions (as a reactant in HXK\_c, HXKfru\_c, ATPu\_c and as a product in PYK\_c, AK\_c and as a modifier in PYK\_c, HXK\_c, AK\_c, HXKfru\_c, ATPu\_c).

$$\frac{d}{dt}ATP_{c} = v_{2} + v_{17} - v_{13} - v_{19} - v_{36}$$
(139)

## 7.19 Species NADP\_g

Name NADP\_g

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

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).

$$\frac{d}{dt}NADP_{-g} = |v_{14}| - |v_{4}| - |v_{29}|$$
 (140)

## 7.20 Species \_6PG\_g

Name \_6PG\_g

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

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 PGI\_g, PGI\_g, \_6PGDH\_g, PGL\_g).

$$\frac{d}{dt} - 6PG - g = |v_{32}| - |v_{29}| \tag{141}$$

## **7.21 Species** C02\_c

Name CO2\_c

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

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:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{CO2}_{-}\mathrm{c} = 0 \tag{142}$$

## 7.22 Species Rul5P\_c

Name Rul5P\_c

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

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).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Rul5P}_{-}c = |v_{26}| - |v_{27}| \tag{143}$$

## 7.23 Species \_6PG\_c

Name \_6PG\_c

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

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).

$$\frac{d}{dt} - 6PG_{-}c = v_{23} - v_{26} \tag{144}$$

## 7.24 Species Rul5P\_g

Name Rul5P\_g

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

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 PPI\_g, \_6PGDH\_g).

$$\frac{d}{dt}Rul5P_{-}g = |v_{29}| - |v_{28}|$$
 (145)

## 7.25 Species Glc6P\_c

Name Glc6P\_c

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

This species takes part in eight 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, HXKfru\_c, HXKfru\_c).

$$\frac{d}{dt}Glc6P_{-}c = |v_{13}| - |v_{7}| - |v_{16}|$$
(146)

## 7.26 Species Rib5P\_c

Name Rib5P\_c

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

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:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Rib5P}_{-}c = 0 \tag{147}$$

## 7.27 Species \_13BPGA\_g

Name \_13BPGA\_g

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

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).

$$\frac{d}{dt} - 13BPGA_{-}g = |v_{39}| - |v_{34}| \tag{148}$$

## 7.28 Species Glc\_c

Name Glc\_c

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

This species takes part in ten 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, HXKfru\_c, HXKfru\_c, GlcT\_g, GlcT\_c).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Glc}_{-}\mathrm{c} = |v_{16}| + |v_{31}| - |v_{13}| - |v_{30}| \tag{149}$$

## 7.29 Species Rib5P\_g

Name Rib5P\_g

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

This species takes part in four reactions (as a reactant in RK\_g and as a product in PPI\_g and as a modifier in RK\_g, PPI\_g).

$$\frac{d}{dt}Rib5P_{-}g = |v_{28}| - |v_{10}| \tag{150}$$

## 7.30 Species Glc\_g

Name Glc\_g

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

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 HXK\_g, HXKfru\_g, HXKfru\_g, GlcT\_g).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Glc}_{-g} = v_{30} - v_{9} \tag{151}$$

## 7.31 Species Glc\_e

Name Glc\_e

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

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:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Glc}_{-}\mathrm{e} = 0 \tag{152}$$

### 7.32 Species NADPH\_g

Name NADPH\_g

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

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).

$$\frac{d}{dt}NADPH_{g} = |v_{4}| + |v_{29}| - |v_{14}|$$
 (153)

## 7.33 Species Rib\_g

Name Rib\_g

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Rib}_{-}\mathrm{g} = 0\tag{154}$$

## 7.34 Species Pyr\_c

Name Pyr\_c

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

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).

$$\frac{\mathrm{d}}{\mathrm{d}t} \mathrm{Pyr}_{\mathbf{c}} c = |v_2| - |v_6| \tag{155}$$

## 7.35 Species Pyr\_e

Name Pyr\_e

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

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:

$$\frac{\mathrm{d}}{\mathrm{d}t} \mathrm{Pyr}_{-} \mathbf{e} = 0 \tag{156}$$

## 7.36 Species NAD\_g

Name NAD\_g

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

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).

$$\frac{d}{dt}NAD_{-}g = v_{35} - v_{39}$$
 (157)

## **7.37 Species** Fru16BP\_g

Name Fru16BP\_g

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

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).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Fru}16\mathrm{BP}_{-}\mathrm{g} = |v_3| - |v_{38}| \tag{158}$$

## 7.38 Species GA3P\_g

Name GA3P\_g

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

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).

$$\frac{d}{dt}GA3P_{-}g = |v_1| + |v_{38}| - |v_{39}|$$
 (159)

## 7.39 Species Gly\_e

Name Gly\_e

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

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:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Gly}_{-}\mathrm{e} = 0 \tag{160}$$

## 7.40 Species TSH2\_c

Name TSH2\_c

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

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).

$$\frac{d}{dt}TSH2_c = v_{33} - v_{20}$$
 (161)

#### **7.41 Species** C02\_g

Name CO2\_g

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

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:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{CO2}_{-\mathrm{g}} = 0\tag{162}$$

## 7.42 Species Gly3P\_c

Name Gly3P\_c

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

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).

$$\frac{d}{dt}Gly3P_{-}c = |v_{21}| - |v_{40}|$$
 (163)

## 7.43 Species Gly3P\_g

Name Gly3P\_g

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

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).

$$\frac{d}{dt}Gly3P_{-}g = |v_{35}| - |v_{21}| - |v_{37}|$$
(164)

## 7.44 Species \_6PGL\_c

Name \_6PGL\_c

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

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).

$$\frac{d}{dt} - 6PGL_c = v_7 - v_{23}$$
 (165)

## 7.45 Species TS2\_c

Name TS2\_c

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

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).

$$\frac{d}{dt}TS2_{-}c = |v_{20}| - |v_{33}| \tag{166}$$

## 7.46 Species \_6PGL\_g

Name \_6PGL\_g

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

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).

$$\frac{d}{dt} - 6PGL_g = |v_4| - |v_{32}| \tag{167}$$

## 7.47 Species PEP\_c

Name PEP\_c

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

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).

$$\frac{\mathrm{d}}{\mathrm{d}t} \mathrm{PEP}_{-c} = |v_8| - |v_2| \tag{168}$$

## 7.48 Species AMP\_g

Name AMP\_g

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

This species takes part in four reactions (as a product in AK\_g and as a modifier in AK\_g, ALD\_g, ALD\_g).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{AMP}_{-}\mathrm{g} = v_{25} \tag{169}$$

## 7.49 Species \_3PGA\_g

Name \_3PGA\_g

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

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).

$$\frac{d}{dt} - 3PGA - g = |v_{34}| - |v_{11}| \tag{170}$$

## 7.50 Species AMP\_c

Name AMP\_c

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{AMP}_{-}\mathrm{c} = |v_{17}| \tag{171}$$

## 7.51 Species NADH\_g

Name NADH\_g

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

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).

$$\frac{d}{dt}NADH_{-}g = |v_{39}| - |v_{35}|$$
 (172)

# 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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