# **SBML Model Report**

# Model name: "Achcar2012 - Glycolysis in bloodstream form T. brucei"



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<sup>1</sup> and Lukas Endler<sup>2</sup> at November 20<sup>th</sup> 2012 at 6:36 p.m. and last time modified at September third 2014 at 4:23 p.m. Table 1 shows an overview of the quantities of all components of this model.

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

Element	Quantity	Element	Quantity
compartment types	0	compartments	3
species types	0	species	31
events	0	constraints	0
reactions	23	function definitions	5
global parameters	0	unit definitions	5
rules	0	initial assignments	0

#### **Model Notes**

Achcar2012 - Glycolysis in bloodstream form T. brucei

Kinetic models of metabolism require quantitative knowledge of detailed kinetic parameters. However, the knowledge about these parameters is often uncertain. An analysis of the effect of

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parameter uncertainties on a particularly well defined example of a quantitative metablic model, the model of glycolysis in bloodstream form Trypanosoma brucei, has been presented here.

This model is described in the article:Dynamic modelling under uncertainty: the case of Trypanosoma brucei energy metabolism. Achcar F, Kerkhoven EJ; SilicoTryp Consortium, Bakker BM, Barrett MP, Breitling R.PLoS Comput Biol. 2012 Jan; 8(1):e1002352.

Abstract:

Kinetic models of metabolism require detailed knowledge of kinetic parameters. However, due to measurement errors or lack of data this knowledge is often uncertain. The model of glycolysis in the parasitic protozoan Trypanosoma brucei is a particularly well analysed example of a quantitative metabolic model, but so far it has been studied with a fixed set of parameters only. Here we evaluate the effect of parameter uncertainty. In order to define probability distributions for each parameter, information about the experimental sources and confidence intervals for all parameters were collected. We created a wiki-based website dedicated to the detailed documentation of this information: the SilicoTryp wiki (http://silicotryp.ibls.gla.ac.uk/wiki/Glycolysis). Using information collected in the wiki, we then assigned probability distributions to all parameters of the model. This allowed us to sample sets of alternative models, accurately representing our degree of uncertainty. Some properties of the model, such as the repartition of the glycolytic flux between the glycerol and pyruvate producing branches, are robust to these uncertainties. However, our analysis also allowed us to identify fragilities of the model leading to the accumulation of 3-phosphoglycerate and/or pyruvate. The analysis of the control coefficients revealed the importance of taking into account the uncertainties about the parameters, as the ranking of the reactions can be greatly affected. This work will now form the basis for a comprehensive Bayesian analysis and extension of the model considering alternative topologies.

This model is hosted on BioModels Database and identified by: MODEL1209130000 .

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

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#### 2 Unit Definitions

This is an overview of five unit definitions.

2.1 Unit volume

Definition µl

2.2 Unit length

**Definition** m

#### 2.3 Unit substance

**Definition** nmol

# 2.4 Unit time

**Definition** 60 s

#### 2.5 Unit area

Definition  $m^2$ 

# 3 Compartments

This model contains three compartments.

Table 2: Properties of all compartments.

			1	1			
Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
cytosol	cytosol		3	5.4549	μl	<b></b>	
glycosome	glycosome		3	0.2451	μl	$\overline{\mathbf{Z}}$	
default	default		3	1	litre		

# 3.1 Compartment cytosol

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

Name cytosol

# 3.2 Compartment glycosome

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

Name glycosome

# 3.3 Compartment default

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

Name default

# 4 Species

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

Table 3: Properties of each species.

Id	Name	Compartment	Derived Unit	Constant	Boundary
					Condi-
					tion
_2PGA_c	_2PGA_c	cytosol	$nmol \cdot \mu l^{-1}$		
$\mathtt{ATP}_{-}\mathtt{g}$	$ATP_{-}g$	glycosome	$nmol \cdot \mu l^{-1}$	$\Box$	
$ATP_c$	ATP_c	cytosol	$n mol \cdot \mu l^{-1}$		
$Pyr_c$	Pyr_c	cytosol	$n mol \cdot \mu l^{-1}$	$\Box$	
DHAP_c	DHAP_c	cytosol	$n mol \cdot \mu l^{-1}$		$\Box$
Pyr_e	Pyr_e	default	$n mol \cdot \mu l^{-1}$		$\checkmark$
Gly3P_c	Gly3P_c	cytosol	$n mol \cdot \mu l^{-1}$		
$DHAP_g$	$DHAP_{-}g$	glycosome	$n mol \cdot \mu l^{-1}$		$\Box$
$\mathtt{NAD}_{-}\mathtt{g}$	$NAD_{-}g$	glycosome	$n mol \cdot \mu l^{-1}$		$\Box$
${ t Glc6P\_g}$	Glc6P_g	glycosome	$n \text{mol} \cdot \mu l^{-1}$		$\Box$
Fru16BP_g	Fru16BP_g	glycosome	$n \text{mol} \cdot \mu l^{-1}$		$\Box$
ADP_c	$ADP_c$	cytosol	$n mol \cdot \mu l^{-1}$		$\Box$
_3PGA_c	_3PGA_c	cytosol	$n mol \cdot \mu l^{-1}$		$\Box$
$Gly_g$	$Gly_g$	glycosome	$n mol \cdot \mu l^{-1}$		$\Box$
Fru6P_g	Fru6P_g	glycosome	$n mol \cdot \mu l^{-1}$		$\Box$
${\tt Gly\_e}$	Gly_e	default	$n mol \cdot \mu l^{-1}$		$ \mathbf{Z} $
_3PGA_g	_3PGA_g	glycosome	$n mol \cdot \mu l^{-1}$		$\Box$
${ t Gly\_c}$	$Gly\_c$	cytosol	$n \text{mol} \cdot \mu l^{-1}$		$\Box$
Pi_g	Pi_g	glycosome	$n mol \cdot \mu l^{-1}$		
AMP_c	$AMP_c$	cytosol	$nmol \cdot \mu l^{-1}$	$\Box$	
02_c	O2_c	default	$nmol \cdot \mu l^{-1}$	$\square$	

Id	Name	Compartment	Derived Unit	Constant	Boundary Condi- tion
GA3P_g	GA3P_g	glycosome	$nmol \cdot \mu l^{-1}$		$\Box$
Gly3P_g	Gly3P_g	glycosome	$nmol \cdot \mu l^{-1}$		$\Box$
$ADP_g$	$ADP_{-}g$	glycosome	$nmol \cdot \mu l^{-1}$		$\Box$
PEP_c	PEP_c	cytosol	$nmol \cdot \mu l^{-1}$		$\Box$
$\mathtt{AMP}_{-}\mathtt{g}$	$AMP_{-}g$	glycosome	$nmol \cdot \mu l^{-1}$		$\Box$
_13BPGA_g	_13BPGA_g	glycosome	$nmol \cdot \mu l^{-1}$		$\Box$
$Glc_c$	Glc_c	cytosol	$nmol \cdot \mu l^{-1}$		$\Box$
Glc_e	Glc_e	default	$nmol \cdot \mu l^{-1}$		
Glc_g	Glc_g	glycosome	$nmol \cdot \mu l^{-1}$		$\Box$
$\mathtt{NADH}_{-}\mathtt{g}$	$NADH_g$	glycosome	$nmol \cdot \mu l^{-1}$		

# 5 Function definitions

This is an overview of five function definitions.

#### 5.1 Function definition mass\_action\_rev

Name mass\_action\_rev

Arguments k1, S, k2, P

**Mathematical Expression** 

$$k1 \cdot S - k2 \cdot P \tag{1}$$

#### **5.2 Function definition VAK**

Name vAK

**Arguments** ADP, AMP, ATP, k1, k2

**Mathematical Expression** 

$$k1 \cdot ADP^2 - AMP \cdot ATP \cdot k2$$
 (2)

# 5.3 Function definition v1sub1prod

Name v1sub1prod

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

**Mathematical Expression** 

$$\frac{V f max \cdot S \cdot \left(1 - \frac{P}{Keq \cdot S}\right)}{Ks \cdot \left(1 + \frac{S}{Ks} + \frac{P}{Kp}\right)}$$
(3)

#### 5.4 Function definition v1sub

Name v1sub

**Arguments** Vfmax, S, Ks

**Mathematical Expression** 

$$\frac{\text{Vfmax} \cdot S}{\text{Ks} \cdot \left(1 + \frac{S}{\text{Ks}}\right)} \tag{4}$$

# **5.5 Function definition** v2sub2prod

Name v2sub2prod

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

**Mathematical Expression** 

$$\frac{V f max \cdot S1 \cdot S2 \cdot \left(1 - \frac{P1 \cdot P2}{Keq \cdot S1 \cdot S2}\right)}{Ks1 \cdot Ks2 \cdot \left(1 + \frac{S2}{Ks2} + \frac{P2}{Kp2}\right) \cdot \left(1 + \frac{S1}{Ks1} + \frac{P1}{Kp1}\right)}$$
 (5)

# **6 Reactions**

This model contains 23 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

N⁰	Id	Name	Reaction Equation	SBO
1	GlyT_g	GlyT_g	$Gly\_g \xrightarrow{Gly\_g, Gly\_c} Gly\_c$	
2	PYK_c	PYK_c	$PEP_{-c} + ADP_{-c} \xrightarrow{ADP_{-c}, PEP_{-c}, ATP_{-c}} Pyr_{-c} +$	
			ATP_c	
3	${\tt GlyT\_c}$	GlyT_c	$Gly\_c \xrightarrow{Gly\_e} Gly\_e$	
4	GlcT_g	GlcT_g	$Glc\_c \xrightarrow{Glc\_c, Glc\_g} Glc\_g$	
5	PyrT_c	PyrT_c	$Pyr_c \xrightarrow{Pyr_c} Pyr_e$	
6	${ t GlcT_c}$	GlcT_c	$Glc_e \xrightarrow{Glc_e, Glc_c} Glc_c$	
7	PFK_g	PFK_g	$ATP_g + Fru6P_g \xrightarrow{ATP_g, Fru6P_g, Fru16BP_g} Fru1$	6BP_g+
			ADP_g	
8	ENO_c	ENO_c	_2PGA_c <del>2PGA_c, PEP_c</del> PEP_c	
9	HXK_g	HXK_g	ATPg + Glcg $ATPg$ , $Glcg$ , $Glc6Pg$ , $ADPg$ $Glc$	6P_g+
	G	<u> </u>	ADP_g	
10	_3PGAT_g	_3PGAT_g	_3PGA_g <del>3PGA_g</del> , _3PGA_c3PGA_c	
11	PGK_g	PGK_g	$_{13BPGA\_g} + ADP\_g \xrightarrow{_{13BPGA\_g}, ADP\_g, _{_{23PGA\_g}}}$	$\underline{g, ATP\_g}$ _3PGA_g
			ATP_g	
12	PGAM_c	PGAM_c	_3PGA_c <del>3PGA_c, _2PGA_c</del> _2PGA_c	

No	Id	Name	Reaction Equation	SBO
13	G3PDH_g	G3PDH_g	NADH_g+DHAP_g DHAP_g, NADH_g, Gly3P_g, N	NAD_g Gly3P_g+
14	ATPu_c	ATPu_c	$ \begin{array}{c} \text{NAD\_g} \\ \text{ATP\_c}, & \xrightarrow{\text{ADP\_c}} & \text{ADP\_c} \end{array} $	
15	GK_g	GK_g	$Gly3Pg + ADPg \xrightarrow{Gly3Pg, ADPg, Glyg, ATPg} Gly3Pg \xrightarrow{Gly3Pg, ADPg, Glyg, ADPg} Gly3Pg \xrightarrow{Gly3Pg, ADPg, Glyg, ATPg} Gly3Pg \xrightarrow{Gly3Pg, ADPg, Glyg, ADPg} Gly3Pg \xrightarrow{Gly3Pg, ADPg} Gly3Pg \xrightarrow{Gly3Pg} Gly3Pg Gly3P$	$\mathrm{Gly}\mathrm{g}+$
	C	Ç	ATP_g Fru16BP_g ATP_g, ADP_g, AMP_g, Fru16BP_g, GA	
16	ALD_g	ALD_g	Fru16BP_g This sylventy and the sylventy	
17	AK_c	AK_c	$2 \text{ ADP\_c}, \frac{\text{ADP\_c}, \text{AMP\_c}, \text{ATP\_c}}{\text{AMP\_c} + \text{ATP\_c}} \text{ AMP\_c} + \text{ATP\_c}$	
	PGI_g	PGI_g	Glc6P_g Glc6P_g, Fru6P_g Fru6P_g	
19	GAPDH_g	GAPDH_g	GA3P_g + NAD_g + Pi_g GA3P_g, NAD_g, _13BPGA_g, NADH_g NADH	T ~ !
			_13BPGA_g	ng +
20	$AK_{-}g$	$AK_{-}g$	$2 \text{ ADP-g} \xrightarrow{\text{ADP-g, AMP-g, ATP-g}} \text{AMP-g+ATP-g}$	IAD .
21	$\mathtt{GDA}_{-}\mathtt{g}$	GDA_g	Gly3P_g+DHAP_c Gly3P_g, DHAP_c, Gly3P_c, DH DHAP_g	$\frac{\text{IAP}_g}{\text{Gly3P}_c} +$
22	GPO_c	GPO_c	Gly3P_c Gly3P_c DHAP_c	
23	TPI_g	TPI_g	$DHAP\_g \xrightarrow{DHAP\_g, GA3P\_g} GA3P\_g$	

# **6.1 Reaction** GlyT\_g

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

Name GlyT\_g

# **Reaction equation**

$$Gly\_g \xrightarrow{Gly\_g, Gly\_c} Gly\_c$$
 (6)

#### Reactant

Table 5: Properties of each reactant.

Id	Name	SBO
Gly_g	$Gly_{-}g$	

#### **Modifiers**

Table 6: Properties of each modifier.

Id	Name	SBO
Gly_g Gly_c	Gly_g Gly_c	

#### **Product**

Table 7: Properties of each product.

Id	Name	SBO
Gly_c	Gly_c	

#### **Kinetic Law**

$$v_1 = \text{mass\_action\_rev} (\text{GlyT\_g\_k}, [\text{Gly\_g}], \text{GlyT\_g\_k}, [\text{Gly\_c}])$$
 (7)

mass\_action\_rev 
$$(k1, S, k2, P) = k1 \cdot S - k2 \cdot P$$
 (8)

Table 8: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
GlyT_g_k	GlyT_g_k	9000.0	Ø

#### 6.2 Reaction PYK\_c

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

#### Name PYK\_c

# **Reaction equation**

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

$$(9)$$

#### **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	
$PEP_{-}c$	PEP_c	
$ATP_c$	ATP_c	

#### **Products**

Table 11: Properties of each product.

Id	Name	SBO
Pyr_c ATP_c	Pyr_c ATP_c	

#### **Kinetic Law**

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

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

Table 12: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
PYK_c_Vmax	PYK_c_Vmax		1020.000		<b>✓</b>
PYK_c_KmPEP	PYK_c_KmPEP		0.340		<b>Z</b>
PYK_c_KiATP	PYK_c_KiATP		0.570		$\overline{\mathbf{Z}}$
$PYK_c_KiADP$	PYK_c_KiADP		0.640		
$PYK_c_n$	PYK_c_n		2.500		
$PYK_c_KmADP$	PYK_c_KmADP		0.114		

# 6.3 Reaction GlyT\_c

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

Name GlyT\_c

#### **Reaction equation**

$$Gly_c \xrightarrow{Gly_c, Gly_e} Gly_e$$
 (11)

#### Reactant

Table 13: Properties of each reactant.

Id	Name	SBO
Gly_c	$Gly\_c$	

#### **Modifiers**

Table 14: Properties of each modifier.

Id	Name	SBO
Gly_c	Gly_c	
${ t Gly_e}$	Gly_e	

#### **Product**

Table 15: Properties of each product.

Id	Name	SBO
Gly_e	Gly_e	

#### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{3} = GlyT\_c\_k \cdot ([Gly\_c] - [Gly\_e]) + \frac{GlyT\_c\_Vmax \cdot ([Gly\_c] - [Gly\_e])}{GlyT\_c\_KmGly \cdot \left(1 + \frac{[Gly\_c]}{GlyT\_c\_KmGly}\right) \cdot \left(1 + \frac{[Gly\_e]}{GlyT\_c\_KmGly}\right)} \tag{12}$$

Table 16: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
$GlyT_c_Vmax$	GlyT_c_Vmax		85.00		
${ t GlyT_c\_KmGly}$	GlyT_c_KmGly		0.17		
GlyT_c_k	GlyT_c_k		9.00		$\blacksquare$

# **6.4 Reaction** GlcT\_g

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

Name GlcT\_g

#### **Reaction equation**

$$Glc\_c \xrightarrow{Glc\_c, Glc\_g} Glc\_g$$
 (13)

#### Reactant

Table 17: Properties of each reactant.

Id	Name	SBO
Glc_c	Glc_c	

#### **Modifiers**

Table 18: Properties of each modifier.

Id	Name	SBO
Glc_c	Glc_c	
${\tt Glc\_g}$	$Glc_g$	

#### **Product**

Table 19: Properties of each product.

Id	Name	SBO
Glc_g	Glc_g	

#### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_4 = \text{mass\_action\_rev} (\text{GlcT\_g\_k}, [\text{Glc\_c}], \text{GlcT\_g\_k}, [\text{Glc\_g}])$$
 (14)

$$mass\_action\_rev(k1, S, k2, P) = k1 \cdot S - k2 \cdot P \tag{15}$$

Table 20: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
GlcT_g_k	GlcT_g_k		250000.0		

# 6.5 Reaction PyrT\_c

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

Name  $PyrT_c$ 

# **Reaction equation**

$$Pyr_{-c} \stackrel{Pyr_{-c}}{\rightleftharpoons} Pyr_{-e}$$
 (16)

#### Reactant

Table 21: Properties of each reactant.

Id	Name	SBO
Pyr_c	Pyr_c	

#### **Modifier**

Table 22: Properties of each modifier.

Id	Name	SBO
Pyr_c	Pyr_c	

#### **Product**

Table 23: Properties of each product.

Id	Name	SBO
Pyr_e	Pyr_e	

#### **Kinetic Law**

$$v_5 = v1sub(PyrT_cVmax, [Pyr_c], PyrT_cKmPyr)$$
(17)

$$v1sub\left(Vfmax,S,Ks\right) = \frac{Vfmax \cdot S}{Ks \cdot \left(1 + \frac{S}{Ks}\right)} \tag{18}$$

Table 24: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
PyrT_c_Vmax	PyrT_c_Vmax		200.00		$\overline{Z}$
PyrT_c_KmPyr	PyrT_c_KmPyr		1.96		Ø

#### 6.6 Reaction GlcT\_c

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

Name GlcT\_c

# **Reaction equation**

$$Glc_e \xrightarrow{Glc_e, Glc_c} Glc_c$$
 (19)

#### Reactant

Table 25: Properties of each reactant.

Id	Name	SBO
Glc_e	Glc_e	

#### **Modifiers**

Table 26: Properties of each modifier.

Id	Name	SBO
Glc_e Glc_c		

# **Product**

Table 27: Properties of each product.

Id	Name	SBO
Glc_c	$Glc\_c$	

# **Kinetic Law**

$$v_{6} = \frac{\text{GlcT\_c\_Vmax} \cdot ([\text{Glc\_e}] - [\text{Glc\_c}])}{[\text{Glc\_e}] + [\text{Glc\_c}] + \text{GlcT\_c\_KmGlc} + \frac{[\text{Glc\_e}] \cdot [\text{Glc\_c}] \cdot \text{GlcT\_c\_alpha}}{\text{GlcT\_c\_KmGlc}}}$$
(20)

Table 28: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
${\tt GlcT\_c\_Vmax}$	GlcT_c_Vmax		108.90		
${\tt GlcT\_c\_KmGlc}$	GlcT_c_KmGlc		1.00		
${ t GlcT_c_alpha}$	GlcT_c_alpha		0.75		

# **6.7 Reaction PFK\_g**

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

# Name PFK\_g

# **Reaction equation**

$$ATP\_g + Fru6P\_g \xrightarrow{ATP\_g, Fru6P\_g, Fru16BP\_g} Fru16BP\_g + ADP\_g \tag{21}$$

#### **Reactants**

Table 29: Properties of each reactant.

Id	Name	SBO
ATP_g	ATP_g	
$Fru6P_g$	Fru6P_g	

#### **Modifiers**

Table 30: Properties of each modifier.

Id	Name	SBO
ATP_g	$ATP_{-}g$	
Fru6P_g	Fru6P_g	
Fru16BP_g	Fru16BP_g	

#### **Products**

Table 31: Properties of each product.

Id	Name	SBO
Fru16BP_g	Fru16BP_g	
ADP_g	$ADP_{-}g$	

#### **Kinetic Law**

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

$$= \frac{\left[\text{ATP\_g}\right] \cdot \left[\text{Fru6P\_g}\right] \cdot \text{PFK\_g\_Vmax} \cdot \text{PFK\_g\_Ki1}}{\text{PFK\_g\_KmFru6P} \cdot \text{PFK\_g\_KmATP} \cdot \left(1 + \frac{\left[\text{ATP\_g}\right]}{\text{PFK\_g\_KmATP}}\right) \cdot \left(\left[\text{Fru16BP\_g}\right] + \text{PFK\_g\_Ki1}\right) \cdot \left(1 + \frac{\left[\text{Fru6P\_g}\right]}{\text{PFK\_g\_KmFru6P}} + \frac{\left[\text{Fru6P\_g}\right]}{\text{PFK\_g\_KmFru6P}}\right)}$$

Table 32: Properties of each parameter.

		1			
Id	Name	SBO	Value	Unit	Constant
PFK_g_Vmax	PFK_g_Vmax		1708.000		$   \sqrt{} $
PFK_g_Ki1	PFK_g_Ki1		15.800		
PFK_g-	PFK_g_KmFru6P		0.820		
_KmFru6P					
$PFK_g_KmATP$	PFK_g_KmATP		0.026		
PFK_g_Ki2	PFK_g_Ki2		10.700		$\square$

#### 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**

$$_{2PGA\_c} \xrightarrow{_{2PGA\_c}, PEP\_c} PEP\_c$$
 (23)

#### 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	

Id	Name	SBO
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

$$v_8 = v1sub1prod (ENO\_c\_Vmax, ENO\_c\_Keq, [\_2PGA\_c], ENO\_c\_Km2PGA, [PEP\_c], \\ ENO\_c\_KmPEP)$$
 (24)

$$v1sub1prod\left(Vfmax,Keq,S,Ks,P,Kp\right) = \frac{Vfmax \cdot S \cdot \left(1 - \frac{P}{Keq \cdot S}\right)}{Ks \cdot \left(1 + \frac{S}{Ks} + \frac{P}{Kp}\right)} \tag{25}$$

Table 36: Properties of each parameter.

		I	1		
Id	Name	SBO	Value	Unit	Constant
ENO_c_Vmax	ENO_c_Vmax		598.000		
$ENO\_c\_Keq$	ENO_c_Keq		6.700		
${\tt ENO\_c\_Km2PGA}$	ENO_c_Km2PGA		0.054		
${\tt ENO\_c\_KmPEP}$	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**

$$ATP\_g + Glc\_g \xrightarrow{ATP\_g, Glc\_g, Glc6P\_g, ADP\_g} Glc6P\_g + ADP\_g \tag{26}$$

#### **Reactants**

Table 37: Properties of each reactant.

Id	Name	SBO
ATP_g Glc_g	ATP_g Glc_g	

#### **Modifiers**

Table 38: Properties of each modifier.

Id	Name	SBO
ATP_g	ATP_g	
${ t Glc}_{- t g}$	Glc_g	
${\tt Glc6P\_g}$	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**

$$\nu_{9} = \frac{[\text{ATP\_g}] \cdot [\text{Glc\_g}] \cdot \text{HXK\_g\_Vmax}}{\text{HXK\_g\_KmGlc} \cdot \text{HXK\_g\_KmATP} \cdot \left(1 + \frac{[\text{Glc\_g}]}{\text{HXK\_g\_KmGlc}} + \frac{[\text{Glc6P\_g}]}{\text{HXK\_g\_KmGlc6P}}\right) \cdot \left(1 + \frac{[\text{ATP\_g}]}{\text{HXK\_g\_KmATP}} + \frac{[\text{ADP\_g}]}{\text{HXK\_g\_KmADP}}\right)}$$

Table 40: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
$HXK_g_Vmax$	$HXK_{-}g_{-}Vmax$		1929.000		
$\tt HXK\_g\_KmGlc$	HXK_g_KmGlc		0.100		
$\mathtt{HXK\_g\_KmATP}$	$HXK_g_KmATP$		0.116		

Id	Name	SBO	Value	Unit	Constant
HXK_g_KmADP HXK_g- _KmGlc6P	HXK_g_KmADP HXK_g_KmGlc6P		0.126 12.000		<b>Z</b>

# 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**

$$_{3}PGA_{g} \xrightarrow{_{3}PGA_{g}, _{3}PGA_{c}} _{3}PGA_{c}$$
 (28)

#### 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	
$_{\mathtt{SPGA\_c}}$	_3PGA_c	

#### **Product**

Table 43: Properties of each product.

Id	Name	SBO
_3PGA_c	_3PGA_c	

#### **Kinetic Law**

$$v_{10} = \text{mass\_action\_rev} \left( \_3PGAT\_g\_k, [\_3PGA\_g], \_3PGAT\_g\_k, [\_3PGA\_c] \right)$$
 (29)

$$mass\_action\_rev(k1, S, k2, P) = k1 \cdot S - k2 \cdot P$$
 (30)

Table 44: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
_3PGAT_g_k	_3PGAT_g_k	250.0	

# **6.11 Reaction PGK\_g**

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

Name PGK\_g

# **Reaction equation**

#### **Reactants**

Table 45: Properties of each reactant.

Id	Name	SBO
_13BPGA_g	_13BPGA_g	
ADP_g	ADP_g	

#### **Modifiers**

Table 46: 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 47: Properties of each product.

Id	Name	SBO
_3PGA_g	_3PGA_g	
$\mathtt{ATP}_{-}\mathtt{g}$	$ATP_{-}g$	

#### **Kinetic Law**

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

$$v_{11} = v2sub2prod(PGK\_g\_Vmax, PGK\_g\_Keq, [\_13BPGA\_g], PGK\_g\_Km13BPGA, [ADP\_g], PGK\_g\_KmADP, [\_3PGA\_g], PGK\_g\_Km3PGA, [ATP\_g], PGK\_g\_KmATP) \eqno(32)$$

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

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

$$(33)$$

Table 48: Properties of each parameter.

	14010 101111	operers	I F		
Id	Name	SBO	Value	Unit	Constant
PGK_g_Vmax	PGK_g_Vmax		2862.000		
$PGK_g_Keq$	PGK_g_Keq		3332.000		
PGK_g-	PGK_g-		0.003		
$_{\tt Km13BPGA}$	_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		<u> </u>

# 6.12 Reaction PGAM\_c

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

Name PGAM\_c

#### **Reaction equation**

$$_{2}PGA_{c} \xrightarrow{2}PGA_{c} -_{2}PGA_{c}$$
 (34)

#### Reactant

Table 49: Properties of each reactant.

Id	Name	SBO
_3PGA_c	_3PGA_c	

#### **Modifiers**

Table 50: Properties of each modifier.

Id	Name	SBO
_3PGA_c	_3PGA_c	
_2PGA_c	_2PGA_c	

#### **Product**

Table 51: Properties of each product.

Id	Name	SBO
_2PGA_c	_2PGA_c	

#### **Kinetic Law**

$$v_{12} = v1sub1prod(PGAM\_c\_Vmax, PGAM\_c\_Keq, [\_3PGA\_c], PGAM\_c\_Km3PGA, \\ [\_2PGA\_c], PGAM\_c\_Km2PGA)$$
 (35)

$$v1sub1prod\left(Vfmax,Keq,S,Ks,P,Kp\right) = \frac{Vfmax \cdot S \cdot \left(1 - \frac{P}{Keq \cdot S}\right)}{Ks \cdot \left(1 + \frac{S}{Ks} + \frac{P}{Kp}\right)} \tag{36}$$

Table 52: Properties of each parameter.

		•			
Id	Name	SBO	Value	Unit	Constant
PGAM_c_Vmax	PGAM_c_Vmax		225.000		lacksquare
$PGAM_c_Keq$	PGAM_c_Keq		0.185		
PGAM_c-	PGAM_c-		0.150		
$_{ m L}$ Km ${ m 3PGA}$	_Km3PGA				

Id	Name	SBO	Value	Unit	Constant
PGAM_c- Km2PGA	PGAM_c- _Km2PGA		0.160		Ø

# 6.13 Reaction G3PDH\_g

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

Name G3PDH\_g

# **Reaction equation**

$$NADH_{-}g + DHAP_{-}g \xrightarrow{DHAP_{-}g, \ NADH_{-}g, \ Gly3P_{-}g, \ NAD_{-}g} Gly3P_{-}g + NAD_{-}g \qquad (37)$$

#### **Reactants**

Table 53: Properties of each reactant.

Id	Name	SBO
NADH_g	NADH_g	
$DHAP_g$	DHAP_g	

#### **Modifiers**

Table 54: Properties of each modifier.

Id	Name	SBO
DHAP_g	DHAP_g	
$NADH_g$	$NADH_{-}g$	
Gly3P_g	Gly3P_g	
$NAD_g$	$NAD_{-}g$	

# **Products**

Table 55: Properties of each product.

Id	Name	SBO
Gly3P_g	Gly3P_g	_
$\mathtt{NAD}_{-}\mathtt{g}$	$NAD_{-}g$	

#### **Kinetic Law**

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

$$\begin{array}{l} v_{13}=v2sub2prod\,(G3PDH\_g\_Vmax,G3PDH\_g\_Keq,[DHAP\_g],G3PDH\_g\_KmDHAP,\\ [NADH\_g],G3PDH\_g\_KmNADH,[Gly3P\_g],G3PDH\_g\_KmGly3P,[NAD\_g],\\ G3PDH\_g\_KmNAD) \end{array} \tag{38}$$

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

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

Table 56: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
G3PDH_g_Vmax	G3PDH_g_Vmax		465.00		lacksquare
G3PDH_g_Keq	G3PDH_g_Keq		2857.00		$\overline{\mathbf{Z}}$
G3PDH_g-	G3PDH_g-		0.10		
_KmDHAP	_KmDHAP				
G3PDH_g-	G3PDH_g-		0.01		
$_{ m L}$ KmNADH	_KmNADH				
G3PDH_g-	G3PDH_g-		2.00		
$_{\tt KmGly3P}$	_KmGly3P				
G3PDH_g-	G3PDH_g-		0.40		
_KmNAD	_KmNAD				

#### 6.14 Reaction ATPu\_c

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

Name ATPu\_c

# **Reaction equation**

$$ATP_{-}c \xrightarrow{ATP_{-}c, ADP_{-}c} ADP_{-}c$$

$$(40)$$

#### Reactant

Table 57: Properties of each reactant.

Id	Name	SBO
ATP_c	ATP_c	

#### **Modifiers**

Table 58: Properties of each modifier.

Id	Name	SBO
	ATP_c ADP_c	

#### **Product**

Table 59: Properties of each product.

Id	Name	SBO
ADP_c	$ADP_{-}c$	

# **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{14} = \frac{[\text{ATP\_c}] \cdot \text{ATPu\_c\_k}}{[\text{ADP\_c}]}$$
(41)

Table 60: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
ATPu_c_k	ATPu_c_k	50.0	$ \overline{Z} $

# **6.15 Reaction** $GK_{-}g$

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

# Name $GK_g$

# **Reaction equation**

$$Gly3P\_g + ADP\_g \xrightarrow{Gly3P\_g, ADP\_g, Gly\_g, ATP\_g} Gly\_g + ATP\_g \tag{42}$$

#### **Reactants**

Table 61: Properties of each reactant.

Id	Name	SBO
Gly3P_g ADP_g	Gly3P_g ADP_g	

#### **Modifiers**

Table 62: Properties of each modifier.

Id	Name	SBO
Gly3P_g	Gly3P_g	
$\mathtt{ADP}_{\mathtt{g}}$	$ADP_{-}g$	
$\operatorname{Gly}_{-}\!g$	$Gly_g$	
$ATP_g$	$ATP_{-}g$	

#### **Products**

Table 63: Properties of each product.

Id	Name	SBO
Gly_g ATP_g	Gly_g ATP_g	

#### **Kinetic Law**

$$\begin{aligned} v_{15} &= v2sub2prod(GK\_g\_Vmax, GK\_g\_Keq, [Gly3P\_g], GK\_g\_KmGly3P, [ADP\_g], \\ &GK\_g\_KmADP, [Gly\_g], GK\_g\_KmGly, [ATP\_g], GK\_g\_KmATP) \end{aligned} \tag{43}$$

$$v2sub2prod (Vfmax, Keq, S1, Ks1, S2, Ks2, P1, Kp1, P2, Kp2) = \frac{Vfmax \cdot S1 \cdot S2 \cdot \left(1 - \frac{P1 \cdot P2}{Keq \cdot S1 \cdot S2}\right)}{Ks1 \cdot Ks2 \cdot \left(1 + \frac{S2}{Ks2} + \frac{P2}{Kp2}\right) \cdot \left(1 + \frac{S1}{Ks1} + \frac{P1}{Kp1}\right)}$$
(44)

Table 64: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
GK_g_Vmax	GK_g_Vmax		200.000		$\overline{Z}$
$GK_g_Keq$	GK_g_Keq		$8 \cdot 10^{-4}$		
$GK_g_KmGly3P$	GK_g_KmGly3P		3.830		
$GK_g_KmADP$	$GK_g_KmADP$		0.560		$\square$
${\tt GK\_g\_KmGly}$	$GK_{g}_{Km}Gly$		0.440		
${\tt GK\_g\_KmATP}$	$GK_{g}_{KmATP}$		0.240		$\square$

# **6.16 Reaction** ALD\_g

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

Name ALD\_g

# **Reaction equation**

$$Fru16BP\_g \xleftarrow{ATP\_g,\ ADP\_g,\ AMP\_g,\ Fru16BP\_g,\ GA3P\_g,\ DHAP\_g,\ ATP\_g,\ ADP\_g,\ AMP\_g} (45)$$

#### Reactant

Table 65: Properties of each reactant.

Id	Name	SBO
Fru16BP_g	Fru16BP_g	

# **Modifiers**

Table 66: Properties of each modifier.

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

Id	Name	SBO

# **Products**

Table 67: Properties of each product.

Id	Name	SBO
GA3P_g	GA3P_g	
$DHAP_g$	DHAP_g	

#### **Kinetic Law**

**Derived unit** contains undeclared units

$$\nu_{16} = \frac{ [Fru16BI] }{ ALD\_g\_KmFru16BP \cdot \left(1 + \frac{[ATP\_g]}{ALD\_g\_KiATP} + \frac{[ADP\_g]}{ALD\_g\_KiADP} + \frac{[AMP\_g]}{ALD\_g\_KiAMP} \right) \cdot \left(1 + \frac{[GA3P\_g]}{ALD\_g\_KmGA3P} + \frac{[DHAP\_g]}{ALD\_g\_KmDHAP} + \frac{[DHAP\_g]}{ALD\_g\_KmDP} + \frac{[DHAP\_g]}{ALD\_g\_KmDP} + \frac{[DHAP\_g]}{ALD\_g\_KmDP} + \frac{[DHAP\_g]$$

Table 68: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
ALD_g_Vmax	ALD_g_Vmax		560.000		<b>✓</b>
ALD_g-	ALD_g-		0.009		$\overline{\mathbf{Z}}$
_KmFru16BP	_KmFru16BP				
$ALD_g_KiATP$	ALD_g_KiATP		0.680		$\square$
$ALD\_g\_KiADP$	ALD_g_KiADP		1.510		
$\mathtt{ALD\_g\_KiAMP}$	ALD_g_KiAMP		3.650		$\square$
$ALD\_g\_Keq$	ALD_g_Keq		0.093		$\square$
$\mathtt{ALD\_g\_KmGA3P}$	ALD_g_KmGA3P		0.067		$\square$
$\mathtt{ALD\_g\_KmDHAP}$	$ALD_g_KmDHAP$		0.015		$\square$
$ALD_g_KiGA3P$	ALD_g_KiGA3P		0.098		

#### 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**

$$2ADP_{c} \xrightarrow{ADP_{c}, AMP_{c}, ATP_{c}} AMP_{c} + ATP_{c}$$

$$(47)$$

#### Reactant

Table 69: Properties of each reactant.

Id	Name	SBO
ADP_c	ADP_c	

#### **Modifiers**

Table 70: Properties of each modifier.

Id	Name	SBO
1121 _0	ADP_c	
$AMP_c$	AMP_c	
$\mathtt{ATP}_\mathtt{c}$	ATP_c	

# **Products**

Table 71: Properties of each product.

Id	Name	SBO
AMP_c	AMP_c	
ATP_c	ATP_c	

#### **Kinetic Law**

$$v_{17} = vAK([ADP_c], [AMP_c], [ATP_c], AK_c k1, AK_c k2)$$
 (48)

$$vAK(ADP, AMP, ATP, k1, k2) = k1 \cdot ADP^{2} - AMP \cdot ATP \cdot k2$$
 (49)

Table 72: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
AK_c_k1	AK_c_k1	442.0	
$AK_c_k2$	$AK_c_k2$	1000.0	$\overline{\checkmark}$

# **6.18 Reaction PGI\_g**

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

Name PGI\_g

#### **Reaction equation**

$$Glc6P\_g \xrightarrow{Glc6P\_g, Fru6P\_g} Fru6P\_g$$
 (50)

#### Reactant

Table 73: Properties of each reactant.

Id	Name	SBO
Glc6P_g	Glc6P_g	

#### **Modifiers**

Table 74: Properties of each modifier.

Id	Name	SBO
Glc6P_g	Glc6P_g	_
Fru6P_g	Fru6P_g	

#### **Product**

Table 75: Properties of each product.

Id	Name	SBO
Fru6P_g	Fru6P_g	

#### **Kinetic Law**

$$\begin{aligned} \nu_{18} = v1sub1prod (PGI\_g\_Vmax, PGI\_g\_Keq, [Glc6P\_g], PGI\_g\_KmGlc6P, [Fru6P\_g], \\ PGI\_g\_KmFru6P) \end{aligned} \tag{51}$$

$$v1sub1prod\left(Vfmax,Keq,S,Ks,P,Kp\right) = \frac{Vfmax \cdot S \cdot \left(1 - \frac{P}{Keq \cdot S}\right)}{Ks \cdot \left(1 + \frac{S}{Ks} + \frac{P}{Kp}\right)} \tag{52}$$

Table 76: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
PGI_g_Vmax PGI_g_Keq PGI_g-	PGI_g_Vmax PGI_g_Keq PGI_g_KmGlc6P		1305.00 0.30 0.40		
_KmGlc6P PGI_g- _KmFru6P	PGI_g_KmFru6P		0.12		Ø

# **6.19 Reaction GAPDH\_g**

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

Name GAPDH\_g

# **Reaction equation**

$$GA3P\_g + NAD\_g + Pi\_g \xrightarrow{GA3P\_g, NAD\_g, -13BPGA\_g, NADH\_g} NADH\_g + -13BPGA\_g \tag{53}$$

#### **Reactants**

Table 77: Properties of each reactant.

Id	Name	SBO
${\tt GA3P\_g}$	GA3P_g	
$NAD_g$	$NAD_{-}g$	
Pi_g	Pi_g	

#### **Modifiers**

Table 78: Properties of each modifier.

Id	Name	SBO
GA3P_g	GA3P_g	
$\mathtt{NAD}_{\mathtt{g}}$	$NAD_{-}g$	
$_{ m 1}$ 3BPGA $_{ m g}$	_13BPGA_g	
NADH_g	NADH_g	

#### **Products**

Table 79: Properties of each product.

Id	Name	SBO
NADH_g	NADH_g	
_13BPGA_g	_13BPGA_g	

#### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{19} = v2sub2prod (GAPDH\_g\_Vmax, GAPDH\_g\_Keq, [GA3P\_g], GAPDH\_g\_KmGA3P, \\ [NAD\_g], GAPDH\_g\_KmNAD, [\_13BPGA\_g], GAPDH\_g\_Km13BPGA, [NADH\_g], \\ GAPDH\_g\_KmNADH) \\ (54)$$

$$\begin{aligned} &v2sub2prod\left(Vfmax,Keq,S1,Ks1,S2,Ks2,P1,Kp1,P2,Kp2\right)\\ &=\frac{Vfmax\cdot S1\cdot S2\cdot \left(1-\frac{P1\cdot P2}{Keq\cdot S1\cdot S2}\right)}{Ks1\cdot Ks2\cdot \left(1+\frac{S2}{Ks2}+\frac{P2}{Kp2}\right)\cdot \left(1+\frac{S1}{Ks1}+\frac{P1}{Kp1}\right)} \end{aligned} \tag{55}$$

Table 80: Properties of each parameter

	14010 60.110	pernes e	n cacii para	ameter.	
Id	Name	SBO	Value	Unit	Constant
GAPDH_g_Vmax	GAPDH_g_Vmax		720.900		
$GAPDH_g_Keq$	GAPDH_g_Keq		0.044		
GAPDH_g-	GAPDH_g-		0.150		$\mathbf{Z}$
_KmGA3P	_KmGA3P				
GAPDH_g-	GAPDH_g-		0.450		
_KmNAD	_KmNAD				
GAPDH_g-	GAPDH_g-		0.100		$\square$
_Km13BPGA	_Km13BPGA				
GAPDH_g-	GAPDH_g-		0.020		
_KmNADH	$_{\perp}$ KmNADH				

# 6.20 Reaction AK\_g

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

Name AK\_g

#### **Reaction equation**

$$2 ADP_{-g} \xleftarrow{ADP_{-g}, AMP_{-g}, ATP_{-g}} AMP_{-g} + ATP_{-g}$$
 (56)

#### Reactant

Table 81: Properties of each reactant.

Id	Name	SBO
ADP_g	$ADP_{-}g$	

#### **Modifiers**

Table 82: Properties of each modifier.

Id	Name	SBO
ADP_g	$ADP_{-}g$	
$\mathtt{AMP}_{-}\mathtt{g}$	$AMP_{-}g$	
$\mathtt{ATP}_{-}\mathtt{g}$	$ATP_{-}g$	

# **Products**

Table 83: Properties of each product.

Id	Name	SBO
AMP_g	AMP_g	
$ATP_g$	ATP_g	

#### **Kinetic Law**

$$v_{20} = vAK([ADP_g], [AMP_g], [ATP_g], AK_g_k1, AK_g_k2)$$
 (57)

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

Table 84: Properties of each parameter.

		1 1	
Id	Name	SBO Value Unit	Constant
AK_g_k1	AK_g_k1	442.0	$\square$
$AK_g_k2$	$AK_g_k2$	1000.0	$\mathbf{Z}$

# **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**

$$Gly3P\_g + DHAP\_c \xleftarrow{Gly3P\_g, DHAP\_c, Gly3P\_c, DHAP\_g} Gly3P\_c + DHAP\_g \qquad (59)$$

#### **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	
${\tt Gly3P\_c}$	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**

$$v_{21} = [Gly3P\_g] \cdot [DHAP\_c] \cdot GDA\_g\_k - [Gly3P\_c] \cdot [DHAP\_g] \cdot GDA\_g\_k$$
 (60)

Table 88: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
GDA_g_k	GDA_g_k	600.0	Ø

#### 6.22 Reaction GPO\_c

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

#### Name GPO\_c

# **Reaction equation**

$$Gly3P_{-c} \xrightarrow{Gly3P_{-c}} DHAP_{-c}$$
(61)

#### Reactant

Table 89: Properties of each reactant.

Id	Name	SBO
Gly3P_c	Gly3P_c	

#### **Modifier**

Table 90: Properties of each modifier.

Id	Name	SBO
Gly3P_c	Gly3P_c	

#### **Product**

Table 91: Properties of each product.

Id	Name	SBO
DHAP_c	DHAP_c	

#### **Kinetic Law**

$$v_{22} = v1sub (GPO_cVmax, [Gly3P_c], GPO_cKmGly3P)$$
(62)

$$v1sub\left(Vfmax,S,Ks\right) = \frac{Vfmax \cdot S}{Ks \cdot \left(1 + \frac{S}{Ks}\right)} \tag{63}$$

Table 92: 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>

# **6.23 Reaction TPI\_g**

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

# Name TPI\_g

# **Reaction equation**

$$DHAP\_g \xrightarrow{DHAP\_g, GA3P\_g} GA3P\_g$$
 (64)

#### Reactant

Table 93: Properties of each reactant.

Id	Name	SBO
DHAP_g	DHAP_g	

#### **Modifiers**

Table 94: Properties of each modifier.

Id	Name	SBO
_	DHAP_g GA3P_g	

#### **Product**

Table 95: Properties of each product.

Id	Name	SBO
GA3P_g	GA3P_g	

#### **Kinetic Law**

Derived unit contains undeclared units

$$v_{23} = v1sub1prod (TPI\_g\_Vmax, TPI\_g\_Keq, [DHAP\_g], TPI\_g\_KmDHAP, [GA3P\_g], TPI\_g\_KmGA3P)$$

$$(65)$$

$$v1sub1prod\left(Vfmax,Keq,S,Ks,P,Kp\right) = \frac{Vfmax \cdot S \cdot \left(1 - \frac{P}{Keq \cdot S}\right)}{Ks \cdot \left(1 + \frac{S}{Ks} + \frac{P}{Kp}\right)} \tag{66}$$

Table 96: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
TPI_g_Vmax	TPI_g_Vmax		999.300		Ø
TPI_g_Keq	TPI_g_Keq		0.045		$\square$
$\mathtt{TPI\_g\_KmDHAP}$	$TPI_g_KmDHAP$		1.200		$\square$
TPI_g_KmGA3P	TPI_g_KmGA3P		0.250		

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

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 ENO\_c, PGAM\_c).

$$\frac{\mathrm{d}}{\mathrm{d}t} \cdot 2\mathrm{PGA} \cdot \mathrm{c} = |v_{12}| - |v_{8}| \tag{67}$$

# 7.2 Species ATP\_g

Name ATP\_g

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

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

$$\frac{d}{dt}ATP_{-g} = |v_{11}| + |v_{15}| + |v_{20}| - |v_{7}| - |v_{9}|$$
(68)

#### 7.3 Species ATP\_c

Name ATP\_c

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

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

$$\frac{d}{dt}ATP_{-}c = v_2 + v_{17} - v_{14}$$
 (69)

#### 7.4 Species Pyr\_c

Name Pyr\_c

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

This species takes part in three reactions (as a reactant in PyrT\_c and as a product in PYK\_c and as a modifier in PyrT\_c).

$$\frac{\mathrm{d}}{\mathrm{d}t} \mathrm{Pyr} \cdot \mathbf{c} = |v_2| - |v_5| \tag{70}$$

#### 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).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{DHAP}_{\cdot}c = v_{22} - v_{21} \tag{71}$$

# 7.6 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:

$$\frac{\mathrm{d}}{\mathrm{d}t} \mathrm{Pyr}_{\cdot} \mathbf{e} = 0 \tag{72}$$

# 7.7 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).

$$\frac{d}{dt}Gly3P_{c} = |v_{21}| - |v_{22}| \tag{73}$$

# 7.8 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 G3PDH\_g, TPI\_g and as a product in ALD\_g, GDA\_g and as a modifier in G3PDH\_g, ALD\_g, GDA\_g, TPI\_g).

$$\frac{d}{dt}DHAP_{g} = |v_{16}| + |v_{21}| - |v_{13}| - |v_{23}|$$
(74)

#### 7.9 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).

$$\frac{d}{dt}NAD_{-}g = v_{13} - v_{19}$$
 (75)

# 7.10 Species Glc6P\_g

Name  $Glc6P_g$ 

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Glc6P}_{-g} = |v_9| - |v_{18}| \tag{76}$$

# 7.11 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).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Fru}16\mathrm{BP}_{-g} = v_7 - v_{16} \tag{77}$$

# 7.12 Species ADP\_c

Name ADP\_c

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

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

$$\frac{d}{dt}ADP_{c} = |v_{14}| - |v_{2}| - 2|v_{17}| \tag{78}$$

#### 7.13 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 \_3PGAT\_g, PGAM\_c).

$$\frac{d}{dt} - 3PGA_c c = |v_{10}| - |v_{12}| \tag{79}$$

# 7.14 Species Gly\_g

Name Gly\_g

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Gly}_{-g} = |v_{15}| - |v_1| \tag{80}$$

# 7.15 Species Fru6P\_g

Name Fru6P\_g

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

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).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Fru6P}_{-\mathrm{g}} = |v_{18}| - v_7 \tag{81}$$

#### 7.16 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 GlyT\_c and as a modifier in GlyT\_c), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Gly}_{-}\mathrm{e} = 0 \tag{82}$$

#### 7.17 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).

$$\frac{d}{dt} - 3PGA - g = |v_{11}| - |v_{10}|$$
 (83)

# 7.18 Species Gly\_c

Name Gly\_c

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Gly}_{-}\mathrm{c} = |v_1| - |v_3| \tag{84}$$

# 7.19 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:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Pi}_{-\mathrm{g}} = 0 \tag{85}$$

#### 7.20 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).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{AMP}_{-}\mathrm{c} = |v_{17}| \tag{86}$$

## **7.21 Species** 02\_c

Name O2\_c

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

$$\frac{\mathrm{d}}{\mathrm{d}t}O2_{-}c = 0 \tag{87}$$

#### **7.22 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 ALD\_g, TPI\_g and as a modifier in ALD\_g, GAPDH\_g, TPI\_g).

$$\frac{d}{dt}GA3P_{-}g = v_{16} + v_{23} - v_{19}$$
 (88)

# **7.23** 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 GK\_g, GDA\_g and as a product in G3PDH\_g and as a modifier in G3PDH\_g, GK\_g, GDA\_g).

$$\frac{d}{dt}Gly3P_{-}g = |v_{13}| - |v_{15}| - |v_{21}|$$
(89)

# 7.24 Species ADP\_g

Name ADP\_g

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

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

$$\frac{d}{dt}ADP_{g} = |v_{7}| + |v_{9}| - |v_{11}| - |v_{15}| - 2|v_{20}|$$
(90)

#### 7.25 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).

$$\frac{\mathrm{d}}{\mathrm{d}t} \mathrm{PEP}_{-c} = v_8 - v_2 \tag{91}$$

# 7.26 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 ALD\_g, ALD\_g, AK\_g).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{AMP}_{-g} = v_{20} \tag{92}$$

# 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).

$$\frac{d}{dt} - 13BPGA_{-g} = v_{19} - v_{11}$$
 (93)

# 7.28 Species Glc\_c

Name Glc\_c

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Glc}_{\cdot}\mathrm{c} = |v_6| - |v_4| \tag{94}$$

#### 7.29 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:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Glc}_{-}\mathrm{e} = 0 \tag{95}$$

#### 7.30 Species Glc\_g

Name Glc\_g

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

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 GlcT\_g, HXK\_g).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Glc}_{-g} = |v_4| - |v_9| \tag{96}$$

## 7.31 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).

$$\frac{d}{dt}NADH_{g} = |v_{19}| - |v_{13}| \tag{97}$$

SML2ATEX was developed by Andreas Dräger<sup>a</sup>, Hannes Planatscher<sup>a</sup>, Dieudonné M Wouamba<sup>a</sup>, Adrian Schröder<sup>a</sup>, Michael Hucka<sup>b</sup>, Lukas Endler<sup>c</sup>, Martin Golebiewski<sup>d</sup> and Andreas Zell<sup>a</sup>. Please see http://www.ra.cs.uni-tuebingen.de/software/SBML2LaTeX for more information.

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