SBML Model Report

Model name: "Bakker2001_Glycolysis"



May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 1 format. This model was created by the following three authors: Jacky L Snoep¹, Harish Dharuri² and Lukas Endler³ at October nineth 2008 at 7:54 p.m. and last time modified at April eighth 2016 at 3:30 p.m. Table 1 gives 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	4
species types	0	species	27
events	0	constraints	0
reactions	14	function definitions	0
global parameters	12	unit definitions	6
rules	13	initial assignments	0

Model Notes

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SBML level 2 code generated for the JWS Online project by Jacky Snoep using PySCeS Run this model online at http://jjj.biochem.sun.ac.za

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To cite JWS Online please refer to: Olivier, B.G. and Snoep, J.L. (2004) Web-based modelling using JWS Online, Bioinformatics, 20:2143-2144

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<u>Biomodels Curation</u>: The paper refers to the model equations present in Bakker et al's "Glycolysis in bloodstream from Trypanosoma brucei can be understood in terms of the kinetics of glycolytic enzymes, (Pubmed ID: 9013556), also, the authors claim that some of the modifications in these equations were made based on the experimental results from the paper "Contribution of glucose transport in the control of glycolytic flux in Trypanosoma brucei, (Pubmed ID: 10468568). The model reproduces the various flux values in Fig 3 for 100% TPI activity. It also matches with the values provided in Table 2 of the paper. The model was successfully tested with Copasi and SBML ODE Solver.

The volumes are set to the values containing 1 mg of total protein per microlitre total cell volume. To change the protein concentration use \underline{Vt} , the total cell volume in micro litre per mg protein.

To change the TPI activity use the global parameter TPIact.

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To cite BioModels Database, please use: Li C, Donizelli M, Rodriguez N, Dharuri H, Endler L, Chelliah V, Li L, He E, Henry A, Stefan MI, Snoep JL, Hucka M, Le Novre N, Laibe C (2010) BioModels Database: An enhanced, curated and annotated resource for published quantitative kinetic models. BMC Syst Biol., 4:92.

2 Unit Definitions

This is an overview of eight unit definitions of which two are predefined by SBML and not mentioned in the model.

2.1 Unit substance

Name nanomole

Definition nmol

2.2 Unit volume

Name microlitre

Definition μl

2.3 Unit microlitre_per_mg

Name microlitre_per_mg

Definition $\mu l \cdot mg^{-1}$

2.4 Unit nanomole_per_min_per_mg

Name nanomole_per_min_per_mg

Definition $nmol \cdot (60 \text{ s})^{-1} \cdot mg^{-1}$

2.5 Unit time

Name minute

Definition 60 s

2.6 Unit mM

Name mM

Definition $nmol \cdot \mu l^{-1}$

2.7 Unit area

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

Definition m^2

2.8 Unit length

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

Definition m

3 Compartments

This model contains four compartments.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
tot_cell	total cell		3	5.7	μl		extracellular

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
glycosome	glycosome		3	0.2446	μl		cytosol
cytosol	cytosol		3	5.4554	μl		extracellular
extracellular	extracellular		3	1	litre		

3.1 Compartment tot_cell

This is a three dimensional compartment with a constant size of $5.7 \,\mu l$, which is surrounded by extracellular (extracellular).

Name total cell

3.2 Compartment glycosome

This is a three dimensional compartment with a constant size of $0.2446 \,\mu l$, which is surrounded by cytosol (cytosol).

Name glycosome

3.3 Compartment cytosol

This is a three dimensional compartment with a constant size of $5.4554 \,\mu l$, which is surrounded by extracellular (extracellular).

Name cytosol

3.4 Compartment extracellular

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

Name extracellular

4 Species

This model contains 27 species. The boundary condition of four of these species is set to true so that these species' amount cannot be changed by any reaction. Section 8 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
GlcI	Glucose	tot_cell	$nmol \cdot \mu l^{-1}$		\Box
Pg	Phosphates in Glycosome	glycosome	$nmol \cdot \mu l^{-1}$		\Box
Glc6P	Glucose 6-phosphate	glycosome	$nmol \cdot \mu l^{-1}$		\Box
Fru6P	Fructose 6-phosphate	glycosome	$nmol \cdot \mu l^{-1}$		\Box
Fru16BP	Fructose 1,6-bisphosphate	glycosome	$nmol \cdot \mu l^{-1}$		\Box
DHAP	Dihydroxyacetone phosphate	${ t tot_{ t cell}}$	$nmol \cdot \mu l^{-1}$		\Box
GAP	Glyceraldehyde 3-phosphate	glycosome	$nmol \cdot \mu l^{-1}$		\Box
NAD	NAD	glycosome	$nmol \cdot \mu l^{-1}$		\Box
BPGA13	1,3-bisphosphoglycerate	glycosome	$nmol \cdot \mu l^{-1}$		\Box
NADH	NADH	glycosome	$nmol \cdot \mu l^{-1}$		\Box
Pyr	Pyruvate	cytosol	$nmol \cdot \mu l^{-1}$		\Box
Nb	3-PGA 2-PGA PEP	${ t tot_{ t cell}}$	$nmol \cdot \mu l^{-1}$		\Box
Pc	Phosphates cytosol	cytosol	$nmol \cdot \mu l^{-1}$		
PyrE	Pyruvate external	extracellular	$nmol \cdot \mu l^{-1}$	\Box	
Gly	Glycerol	glycosome	$nmol \cdot \mu l^{-1}$		$ \overline{\mathbf{Z}} $
GlcE	Glucose external	extracellular	$nmol \cdot \mu l^{-1}$		
Gly3P	Glycerol 3-phosphate	${ t tot_{ t cell}}$	$nmol \cdot \mu l^{-1}$		$ \overline{\mathbf{Z}} $
ATPc	ATP cyt.	cytosol	$nmol \cdot \mu l^{-1}$		
ADPc	ADP cyt.	cytosol	$nmol \cdot \mu l^{-1}$		\Box
ATPg	ATP gly.	glycosome	$nmol \cdot \mu l^{-1}$		
ADPg	ADP gly.	glycosome	$nmol \cdot \mu l^{-1}$		

Id	Name	Compartment	Derived Unit	Constant	Boundary Condi- tion
DHAPg	DHAP gly.	glycosome	$nmol \cdot \mu l^{-1}$		\Box
DHAPc	DHAP cyt.	cytosol	$nmol \cdot \mu l^{-1}$		\Box
Gly3Pc	Gy3P c.	cytosol	$nmol \cdot \mu l^{-1}$		\Box
Gly3Pg	Gy3P g.	glycosome	$nmol \cdot \mu l^{-1}$		\Box
PGAg	3-PGA g.	glycosome	$nmol \cdot \mu l^{-1}$		\Box
PEPc	PEP c.	cytosol	$nmol \cdot \mu l^{-1}$		\Box

5 Parameters

This model contains twelve global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vt	tot volume per mg		5.700	$\mu l \cdot mg^{-1}$	\overline{Z}
	protein				
Vc	Vc		0.000	$\mu l \cdot mg^{-1}$	\Box
Vg	Vg		0.000	$\mu l \cdot mg^{-1}$	\Box
TPIact			1.000	dimensionless	
sumAc			3.900	$nmol \cdot \mu l^{-1}$	$ \overline{\mathbf{Z}} $
sumAg			6.000	$nmol \cdot \mu l^{-1}$	$ \overline{\mathscr{L}} $
KeqAK			0.442	dimensionless	$ \overline{\mathbf{Z}} $
Keq_anti			1.000	dimensionless	$\overline{\mathbf{Z}}$
sumc4			45.000	$nmol \cdot \mu l^{-1}$	\overline{Z}
sumc5			5.000	$nmol \cdot \mu l^{-1}$	$\overline{\mathbf{Z}}$
${\tt Keq_PGM}$			0.187	dimensionless	$\overline{\mathbf{Z}}$
Keq_ENO			6.700	dimensionless	$\overline{\mathbf{Z}}$

6 Rules

This is an overview of 13 rules.

6.1 Rule Vc

Rule Vc is an assignment rule for parameter Vc:

$$Vc = \frac{\text{vol}(\text{cytosol}) \cdot Vt}{\text{vol}(\text{tot_cell})} \tag{1}$$

Derived unit $10^{-6} \, l \cdot mg^{-1}$

6.2 Rule Vg

Rule Vg is an assignment rule for parameter Vg:

$$Vg = \frac{\text{vol}(\text{glycosome}) \cdot Vt}{\text{vol}(\text{tot_cell})}$$
 (2)

Derived unit $10^{-6} \, l \cdot mg^{-1}$

6.3 Rule ATPg

Rule ATPg is an assignment rule for species ATPg:

$$\frac{\text{ATPg}}{=\frac{[\text{Pg}] \cdot (1 - 4 \cdot \text{KeqAK}) - \text{sumAg} + \left((\text{sumAg} - (1 - 4 \cdot \text{KeqAK}) \cdot [\text{Pg}])^2 + 4 \cdot (1 - 4 \cdot \text{KeqAK}) \cdot \text{KeqAK} \cdot [\text{Pg}]^2}{2 \cdot (1 - 4 \cdot \text{KeqAK})}$$

6.4 Rule ADPg

Rule ADPg is an assignment rule for species ADPg:

$$ADPg = [Pg] - 2 \cdot [ATPg] \tag{4}$$

6.5 Rule ATPc

Rule ATPc is an assignment rule for species ATPc:

$$\begin{aligned} & \text{ATPc} \\ & = \frac{\left[\text{Pc}\right] \cdot \left(1 - 4 \cdot \text{KeqAK}\right) - \text{sumAc} + \left(\left(\text{sumAc} - \left(1 - 4 \cdot \text{KeqAK}\right) \cdot \left[\text{Pc}\right]\right)^2 + 4 \cdot \left(1 - 4 \cdot \text{KeqAK}\right) \cdot \text{KeqAK} \cdot \left[\text{Pc}\right]^2\right)}{2 \cdot \left(1 - 4 \cdot \text{KeqAK}\right)} \end{aligned}$$

6.6 Rule ADPc

Rule ADPc is an assignment rule for species ADPc:

$$ADPc = [Pc] - 2 \cdot [ATPc] \tag{6}$$

6.7 Rule DHAPc

Rule DHAPc is an assignment rule for species DHAPc:

DHAPc

$$=\frac{\text{sumc5}\cdot\left(1+\frac{\text{Vc}}{\text{Vg}}\right)\cdot\left[\text{DHAP}\right]}{\text{sumc4}+\frac{\text{sumc5}\cdot\text{Vc}}{\text{Vg}}-\left(\left[\text{BPGA13}\right]+2\cdot\left[\text{Fru16BP}\right]+\left[\text{Fru6P}\right]+\left[\text{GAP}\right]+\left[\text{Glc6P}\right]+\left[\text{Pg}\right]\right)}{(7)}$$

6.8 Rule DHAPg

Rule DHAPg is an assignment rule for species DHAPg:

$$DHAPg = \frac{[DHAP] \cdot Vt - [DHAPc] \cdot Vc}{Vg}$$
(8)

Derived unit $nmol \cdot \mu l^{-1}$

6.9 Rule Gly3Pc

Rule Gly3Pc is an assignment rule for species Gly3Pc:

$$Gly3Pc = sumc5 - [DHAPc]$$
 (9)

Derived unit $nmol \cdot \mu l^{-1}$

6.10 Rule Gly3Pg

Rule Gly3Pg is an assignment rule for species Gly3Pg:

$$Gly3Pg = \frac{[Gly3Pc] \cdot [DHAPg]}{Keq_anti \cdot [DHAPc]}$$
(10)

Derived unit $9.9999999999998 \cdot 10^{-10} \text{ mol} \cdot \left(10^{-6} \text{ I}\right)^{-1}$

6.11 Rule Gly3P

Rule Gly3P is an assignment rule for species Gly3P:

$$Gly3P = \frac{[Gly3Pc] \cdot vol (cytosol) + [Gly3Pg] \cdot vol (glycosome)}{vol (tot_cell)}$$
(11)

Derived unit $nmol \cdot \mu l^{-1}$

6.12 Rule PGAg

Rule PGAg is an assignment rule for species PGAg:

$$PGAg = \frac{[Nb] \cdot \left(1 + \frac{Vc}{Vg}\right)}{1 + \frac{(1 + Keq.PGM + Keq.PGM \cdot Keq.ENO) \cdot Vc}{Vg}}$$
(12)

6.13 Rule PEPc

Rule PEPc is an assignment rule for species PEPc:

$$PEPc = Keq_ENO \cdot Keq_PGM \cdot [PGAg]$$
 (13)

Derived unit $nmol \cdot \mu l^{-1}$

7 Reactions

This model contains 14 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 5: Overview of all reactions

N₀	Id	Name	Reaction Equation	SBO
1	vGlcTr	Glucose transport	GlcE ← GlcI	
2	vHK	Hexokinase	$Pg + GlcI \xrightarrow{ATPg, ADPg} Glc6P$	
3	vPGI	Glucose-phosphate isomerase	Glc6P ← Fru6P	
4	vPFK	Phosphofructokinase	$Pg + Fru6P \xrightarrow{ATPg} Fru16BP$	
5	vALD	Aldolase	Fru16BP DHAPg, ATPg, ADPg GAP + DHAP	
6	vTPI	Triosephosphate isomerase	$DHAP \xrightarrow{DHAPg} GAP$	
7	vGAPdh	Glyceraldehyde 3-phosphate dehydrogenase	$GAP + NAD \Longrightarrow NADH + BPGA13$	
8	vGDH	Glycerol 3-phosphate dehydrogenase	$DHAP + NADH \xrightarrow{DHAPg, Gly3Pg} NAD + Gly3P$	
9	vGPO	Glycerol 3-phosphate oxidase	$Gly3P \xrightarrow{Gly3Pc} DHAP$	
10	vPyrTr	Pyruvate transport	$Pyr \longrightarrow PyrE$	
11	vPGK	Phosphoglycerate kinase	$BPGA13 \xrightarrow{ADPg, ATPg, PGAg} Nb + Pg$	
12	vPK	Pyruvate kinase	$Nb \xrightarrow{PEPc, ADPc, ATPc} Pc + Pyr$	
13	vATPase	ATPase	$Pc \xrightarrow{ATPc, ADPc} \emptyset$	
14	vGlyK	Glycerol kinase	$Gly3P \xrightarrow{ADPg, Gly3Pg, ATPg} Pg + Gly$	

7.1 Reaction vGlcTr

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

Name Glucose transport

Reaction equation

$$GlcE \rightleftharpoons GlcI$$
 (14)

Reactant

Table 6: Properties of each reactant.

Id	Name	SBO
GlcE	Glucose external	

Product

Table 7: Properties of each product.

Id	Name	SBO
GlcI	Glucose	

Kinetic Law

Derived unit $9.9999999999998 \cdot 10^{-10} \text{ mol} \cdot (60 \text{ s})^{-1}$

$$v_{1} = \frac{\frac{\text{vol(tot_cell)}}{\text{Vt}} \cdot \text{Vm1} \cdot ([\text{GlcE}] - [\text{GlcI}])}{\text{K1Glc} + [\text{GlcE}] + [\text{GlcI}] + \frac{\text{afac} \cdot [\text{GlcE}] \cdot [\text{GlcI}]}{\text{K1Glc}}}$$
(15)

Table 8: Properties of each parameter.

		1	1		
Id	Name	SBO	Value	Unit	Constant
Vm1			106.20	$\begin{array}{c} \text{nmol} & \cdot & (60 \text{ s})^{-1} & \cdot \\ \text{mg}^{-1} & \end{array}$	
K1Glc			2.00	$nmol \cdot \mu l^{-1}$	
afac			0.75	dimensionless	

7.2 Reaction vHK

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

Name Hexokinase

Reaction equation

$$Pg + GlcI \xrightarrow{ATPg, ADPg} Glc6P$$
 (16)

Reactants

Table 9: Properties of each reactant.

Id	Name	SBO
Pg GlcI	Phosphates in Glycosome Glucose	

Modifiers

Table 10: Properties of each modifier.

Id	Name	SBO
ATPg	ATP gly.	
ADPg	ADP gly.	

Product

Table 11: Properties of each product.

Id	Name	SBO
Glc6P	Glucose 6-phosphate	

Kinetic Law

Derived unit contains undeclared units

$$v_{2} = \frac{\frac{vol(tot_cell)}{Vt} \cdot Vm2 \cdot [GlcI] \cdot [ATPg]}{K2ATPg \cdot K2GlcI \cdot \left(1 + \frac{[Glc6P]}{K2Glc6P} + \frac{[GlcI]}{K2GlcI}\right) \cdot \left(1 + \frac{[ATPg]}{K2ATPg} + \frac{[ADPg]}{K2ADPg}\right)}$$
(17)

Table 12: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vm2			625.000	$\begin{array}{c} nmol & \cdot & (60 \text{ s})^{-1} & \cdot \\ mg^{-1} & \end{array}$	
K2ATPg			0.116	$nmol \cdot \mu l^{-1}$	
K2GlcI			0.100	$nmol \cdot \mu l^{-1}$	
K2Glc6P			12.000	$nmol \cdot \mu l^{-1}$	
K2ADPg			0.126	$nmol \cdot \mu l^{-1}$	

7.3 Reaction vPGI

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

Name Glucose-phosphate isomerase

Reaction equation

$$Glc6P \rightleftharpoons Fru6P$$
 (18)

Reactant

Table 13: Properties of each reactant.

Id	Name	SBO
Glc6P	Glucose 6-phosphate	

Product

Table 14: Properties of each product.

14010 1	Tueste I ii I I eperities er euem producti		
Id	Name	SBO	
Fru6P	Fructose 6-phosphate		

Kinetic Law

Derived unit contains undeclared units

$$v_{3} = \frac{\frac{\text{vol(tot_cell)}}{\text{Vt}} \cdot \text{Vm3} \cdot \left(\frac{[\text{Glc6P}]}{\text{K3Glc6P}} - \frac{[\text{Fru6P}]}{\text{K3Fru6P}}\right)}{1 + \frac{[\text{Glc6P}]}{\text{K3Glc6P}} + \frac{[\text{Fru6P}]}{\text{K3Fru6P}}}$$
(19)

Table 15: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
	- T (dillo				
Vm3		8	348.00	$nmol \cdot (60 s)^{-1} \cdot$	
				mg^{-1}	
K3Glc6P			0.40	$nmol \cdot \mu l^{-1}$	\square
K3Fru6P			0.12	$nmol \cdot \mu l^{-1}$	

7.4 Reaction vPFK

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

Name Phosphofructokinase

Reaction equation

$$Pg + Fru6P \xrightarrow{ATPg} Fru16BP$$
 (20)

Reactants

Table 16: Properties of each reactant.

Tuon	Tuble 10. I toperties of each reactant.			
Id	Name	SBO		
Pg Fru6P	Phosphates in Glycosome Fructose 6-phosphate			

Modifier

Table 17: Properties of each modifier.

Id	Name	SBO
ATPg	ATP gly.	

Product

Table 18: Properties of each product.

Id	Name	SBO
Fru16BP	Fructose 1,6-bisphosphate	

Kinetic Law

Derived unit contains undeclared units

$$v_{4} = \frac{\frac{vol(tot_cell)}{Vt} \cdot K4i1Fru16BP \cdot Vm4 \cdot [Fru6P] \cdot [ATPg]}{K4ATPg \cdot K4Fru6P \cdot (K4i1Fru16BP + [Fru16BP]) \cdot \left(1 + \frac{[Fru16BP]}{K4i2Fru16BP} + \frac{[Fru6P]}{K4Fru6P}\right) \cdot \left(1 + \frac{[ATPg]}{K4ATPg}\right)}$$

Table 19: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
K4i1Fru16E	BP .		15.800	$nmol \cdot \mu l^{-1}$	
Vm4			780.000	$nmol \cdot (60 s)^{-1} \cdot$	
				mg^{-1}	
K4ATPg			0.026	$nmol \cdot \mu l^{-1}$	
K4Fru6P			0.820	$nmol \cdot \mu l^{-1}$	
K4i2Fru16E	3P		10.700	$nmol \cdot \mu l^{-1}$	$ \overline{\mathbf{Z}} $

7.5 Reaction vALD

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

Name Aldolase

Reaction equation

$$Fru16BP \xrightarrow{DHAPg, ATPg, ADPg} GAP + DHAP$$
 (22)

Reactant

Table 20: Properties of each reactant.

Id	Name	SBO
Fru16BP	Fructose 1,6-bisphosphate	

Modifiers

Table 21: Properties of each modifier.

Id	Name	SBO
DHAPg	DHAP gly.	
ATPg	ATP gly.	
ADPg	ADP gly.	

Products

Table 22: Properties of each product.

Id	Name	SBO
GAP DHAP	Glyceraldehyde 3-phosphate Dihydroxyacetone phosphate	

Kinetic Law

Derived unit contains undeclared units

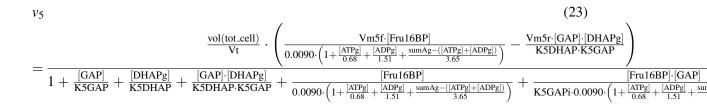


Table 23: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vm5r			219.555	$nmol \cdot (60 s)^{-1} \cdot$	
				mg^{-1}	
K5DHAP			0.015	$n mol \cdot \mu l^{-1}$	
K5GAP			0.067	$nmol \cdot \mu l^{-1}$	$ \overline{\mathscr{L}} $
Vm5f			184.500	$nmol \cdot (60 s)^{-1} \cdot$	
				mg^{-1}	
K5GAPi			0.098	$nmol \cdot \mu l^{-1}$	\blacksquare

7.6 Reaction vTPI

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

Name Triosephosphate isomerase

Reaction equation

$$DHAP \xrightarrow{DHAPg} GAP \tag{24}$$

Reactant

Table 24: Properties of each reactant.

Id	Name	SBO
DHAP	Dihydroxyacetone phosphate	

Modifier

Table 25: Properties of each modifier.

Id	Name	SBO
DHAPg	DHAP gly.	

Product

Table 26: Properties of each product.

Id	Name	SBO
GAP	Glyceraldehyde 3-phosphate	

Kinetic Law

Derived unit contains undeclared units

$$v_{6} = \frac{\frac{\text{vol(tot.cell)}}{\text{Vt}} \cdot \text{TPIact} \cdot \text{Vm6} \cdot \left(\frac{[\text{DHAPg}]}{\text{K6DHAPg}} - \frac{5.7 \cdot [\text{GAP}]}{\text{K6GAP}}\right)}{1 + \frac{[\text{GAP}]}{\text{K6GAP}} + \frac{[\text{DHAPg}]}{\text{K6DHAPg}}}$$
(25)

Table 27: Properties of each parameter.

			r		
Id	Name	SBO V	Value	Unit	Constant
Vm6		8	42.00	$\begin{array}{c} nmol & \cdot & (60 \text{ s})^{-1} & \cdot \\ mg^{-1} & \end{array}$	Ø
K6GAP K6DHAPg				$\begin{array}{l} nmol \cdot \mu l^{-1} \\ nmol \cdot \mu l^{-1} \end{array}$	Z

7.7 Reaction vGAPdh

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

Name Glyceraldehyde 3-phosphate dehydrogenase

Reaction equation

$$GAP + NAD \Longrightarrow NADH + BPGA13 \tag{26}$$

Reactants

Table 28: Properties of each reactant.

Id	Name	SBO
	Glyceraldehyde 3-phosphate NAD	

Products

Table 29: Properties of each product.

	1 1	
Id	Name	SBO
NADH	NADH	
BPGA13	1,3-bisphosphoglycerate	

Kinetic Law

Derived unit contains undeclared units

$$v_{7} = \frac{\text{vol}\left(\text{tot_cell}\right)}{\text{Vt}} \cdot \text{Vm7} \cdot \frac{\text{Vm7f} \cdot \left(\left[\text{GAP}\right] \cdot \frac{\left[\text{NAD}\right]}{\text{K7NAD}} - \frac{\text{Vm7r}}{\text{Vm7f}} \cdot \frac{\frac{\left[\text{BPGA13}\right] \cdot \left[\text{NADH}\right]}{\text{K7BPGA13}}}{\left(1 + \frac{\left[\text{GAP}\right]}{\text{K7GAP}} + \frac{\left[\text{BPGA13}\right]}{\text{K7BPGA13}}\right) \cdot \left(1 + \frac{\left[\text{NAD}\right]}{\text{K7NAD}} + \frac{\left[\text{NADH}\right]}{\text{K7NADH}}\right)}$$
(27)

Table 30: Properties of each parameter.

		•			
Id	Name	SBO	Value	Unit	Constant
Vm7			1.00	dimensionless	\overline{Z}
Vm7f			1470.00	$nmol \cdot (60 s)^{-1} \cdot$	
				mg^{-1}	
K7GAP			0.15	$nmol \cdot \mu l^{-1}$	

Id	Name	SBO	Value	Unit	Constant
K7NAD			0.45	$nmol \cdot \mu l^{-1}$	\overline{Z}
Vm7r			984.90	$nmol \cdot (60 s)^{-1} \cdot$	
				mg^{-1}	
K7BPGA13			0.10	$nmol \cdot \mu l^{-1}$	
K7NADH			0.02	$nmol \cdot \mu l^{-1}$	

7.8 Reaction vGDH

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

Name Glycerol 3-phosphate dehydrogenase

Reaction equation

$$DHAP + NADH \xrightarrow{DHAPg, Gly3Pg} NAD + Gly3P$$
 (28)

Reactants

Table 31: Properties of each reactant.

Id	Name	SBO
	Dihydroxyacetone phosphate	
NADH	NADH	

Modifiers

Table 32: Properties of each modifier.

Id	Name	SBO
DHAPg	DHAP gly.	
Gly3Pg	Gy3P g.	

Products

Table 33: Properties of each product.

Id	Name	SBO
NAD	NAD	
Gly3P	Glycerol 3-phosphate	

Kinetic Law

Derived unit contains undeclared units

$$v_{8} = \frac{\frac{\text{vol(tot_cell)}}{\text{Vt}} \cdot \text{Vm8} \cdot \text{Vm8f} \cdot \left(\frac{[\text{NADH}] \cdot [\text{DHAPg}]}{\text{K8DHAPg} \cdot \text{K8NADH}} - \frac{\text{Vm8r} \cdot [\text{NAD}] \cdot [\text{Gly3Pg}]}{\text{K8Gly3Pg} \cdot \text{K8NAD} \cdot \text{Vm8f}}\right)}{\left(1 + \frac{[\text{NAD}]}{\text{K8NAD}} + \frac{[\text{NADH}]}{\text{K8NADH}}\right) \cdot \left(1 + \frac{[\text{DHAPg}]}{\text{K8DHAPg}} + \frac{[\text{Gly3Pg}]}{\text{K8Gly3Pg}}\right)}$$
(29)

Table 34: Properties of each parameter.

		1			
Id	Name	SBO	Value	Unit	Constant
Vm8			1.00	dimensionless	
Vm8f			533.00	$nmol \cdot (60 s)^{-1} \cdot$	
				mg^{-1}	
K8DHAPg			0.10	$nmol \cdot \mu l^{-1}$	
K8NADH			0.01	$nmol \cdot \mu l^{-1}$	
Vm8r			149.24	$nmol \cdot (60 s)^{-1} \cdot$	
				mg^{-1}	
K8Gly3Pg			2.00	$nmol \cdot \mu l^{-1}$	
K8NAD			0.40	$nmol \cdot \mu l^{-1}$	$ \overline{\mathbf{Z}} $

7.9 Reaction vGPO

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

Name Glycerol 3-phosphate oxidase

Reaction equation

$$Gly3P \xrightarrow{Gly3Pc} DHAP \tag{30}$$

Reactant

Table 35: Properties of each reactant.

Id	Name	SBO
Gly3P	Glycerol 3-phosphate	

Modifier

Table 36: Properties of each modifier.

Id	Name	SBO
Gly3Pc	Gy3P c.	

Product

Table 37: Properties of each product.

Id	Name	SBO
DHAP	Dihydroxyacetone phosphate	

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \frac{\frac{\text{vol(tot_cell)}}{\text{Vt}} \cdot \text{Vm9} \cdot [\text{Gly3Pc}]}{\text{K9Gly3Pc} \cdot 1 + [\text{Gly3Pc}]}$$
(31)

Table 38: Properties of each parameter.

IdNameSBOValueUnitConstantVm9368.0 $nmol \cdot (60 \text{ s})^{-1} \cdot \text$						
mg^{-1}	Id	Name	SBO	Value	Unit	Constant
K9Gly3Pc 1.7 $\text{nmol} \cdot \mu l^{-1}$	Vm9			368.0		\checkmark
	K9Gly3Pc			1.7	$n \text{mol} \cdot \mu l^{-1}$	✓

7.10 Reaction vPyrTr

This is an irreversible reaction of one reactant forming one product.

Name Pyruvate transport

Reaction equation

$$Pyr \longrightarrow PyrE \tag{32}$$

Reactant

Table 39: Properties of each reactant.

Id	Name	SBO
Pyr	Pyruvate	

Product

Table 40: Properties of each product.

Id	Name	SBO
PyrE	Pyruvate external	

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = \frac{\frac{\frac{\text{vol(tot.cell)}}{\text{Vt}} \cdot \text{Vm} 10 \cdot [\text{Pyr}]}{\text{K} 10 \text{Pyr}}}{1 + \frac{[\text{Pyr}]}{\text{K} 10 \text{Pyr}}}$$
(33)

Table 41: Properties of each parameter.

Id	Name	SBO Value	Unit	Constant
Vm10		200.00	$\begin{array}{cc} \text{nmol} & (60 \text{ s})^{-1} \\ \text{mg}^{-1} \end{array}$. 🗹
K10Pyr		1.90	$5 \text{nmol} \cdot \mu l^{-1}$	

7.11 Reaction vPGK

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

Name Phosphoglycerate kinase

Reaction equation

$$BPGA13 \xrightarrow{ADPg, ATPg, PGAg} Nb + Pg$$
 (34)

Reactant

Table 42: Properties of each reactant.

	· z · r · r · p · r · r · r · r · r · r · r	
Id	Name	SBO
BPGA13	1,3-bisphosphoglycerate	

Modifiers

Table 43: Properties of each modifier.

Id	Name	SBO
ADPg	ADP gly.	
ATPg	ATP gly.	
PGAg	3-PGA g.	

Products

Table 44: Properties of each product.

	F F	
Id	Name	SBO
Nb	3-PGA 2-PGA PEP	
Pg	Phosphates in Glycosome	

Kinetic Law

Derived unit contains undeclared units

$$v_{11} = \frac{\frac{\text{vol(tot_cell)}}{\text{Vt}} \cdot \text{Vm}11 \cdot \text{Vm}11f \cdot \left(\frac{\text{Vm}11r \cdot [\text{PGAg}] \cdot [\text{ATPg}]}{\text{K11ATPg} \cdot \text{K11PGA3} \cdot \text{Vm}11f} + \frac{[\text{BPGA13}] \cdot [\text{ADPg}]}{\text{K11ADPg} \cdot \text{K11BPGA13}}\right)}{\left(1 + \frac{[\text{BPGA13}]}{\text{K11BPGA13}} + \frac{[\text{PGAg}]}{\text{K11PGA3}}\right) \cdot \left(1 + \frac{[\text{ATPg}]}{\text{K11ATPg}} + \frac{[\text{ADPg}]}{\text{K11ADPg}}\right)}$$
(35)

Table 45: Properties of each parameter.

$\begin{array}{c ccccccccccccccccccccccccccccccccccc$			1	1		
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Id	Name	SBO	Value	Unit	Constant
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Vm11			1.00	dimensionless	\overline{Z}
Vm11r $18.56 \text{nmol} \cdot (60 \text{ s})^{-1} \cdot \text$	Vm11f			640.00		
$ m mg^{-1}$ K11ATPg $0.29 nmol \cdot \mu l^{-1}$						_
K11ATPg $0.29 \text{ nmol} \cdot \mu l^{-1}$	Vm11r			18.56	` ,	\square
					•	
K11PGA3 $1.62 \text{ nmol} \cdot \mu l^{-1}$	K11ATPg			0.29	$nmol \cdot \mu l^{-1}$	\square
	K11PGA3			1.62	$nmol \cdot \mu l^{-1}$	

Id	Name	SBO	Value	Unit	Constant
K11ADPg K11BPGA13				dimensionless dimensionless	

7.12 Reaction vPK

This is an irreversible reaction of one reactant forming two products influenced by three modifiers

Name Pyruvate kinase

Reaction equation

$$Nb \xrightarrow{PEPc, ADPc, ATPc} Pc + Pyr$$
 (36)

Reactant

Table 46: Properties of each reactant.

Id	Name	SBO
Nb	3-PGA 2-PGA PEP	

Modifiers

Table 47: Properties of each modifier.

Id	Name	SBO
PEPc	PEP c.	
ADPc	ADP cyt.	
ATPc	ATP cyt.	

Products

Table 48: Properties of each product.

Id	Name	SBO
Рс	Phosphates cytosol	
Pyr	Pyruvate	

Kinetic Law

Derived unit contains undeclared units

$$v_{12} = \frac{\frac{\frac{\text{vol(tot.cell)}}{\text{Vt}} \cdot \text{Vm}12 \cdot \left(\frac{\frac{[\text{PEPc}]}{0.34 \cdot \left(1 + \frac{[\text{ADPc}]}{0.64}\right)}\right)^{n12} \cdot [\text{ADPc}]}{\frac{\text{K}12\text{ADP}}{\left(1 + \left(\frac{[\text{PEPc}]}{0.34 \cdot \left(1 + \frac{[\text{ADPc}]}{0.57} + \frac{[\text{ATPc}]}{0.64}\right)}\right)^{n12}\right) \cdot \left(1 + \frac{[\text{ADPc}]}{\text{K}12\text{ADP}}\right)}}$$
(37)

Table 49: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
n12			2.500	dimensionless	\overline{Z}
Vm12			2600.000	$nmol \cdot (60 s)^{-1} \cdot$	\checkmark
				mg^{-1}	
K12ADP			0.114	$nmol \cdot \mu l^{-1}$	\square

7.13 Reaction vATPase

This is an irreversible reaction of one reactant forming no product influenced by two modifiers.

Name ATPase

Reaction equation

$$Pc \xrightarrow{ATPc, ADPc} \emptyset$$
 (38)

Reactant

Table 50: Properties of each reactant.

Id	Name	SBO
Рс	Phosphates cytosol	

Modifiers

Table 51: Properties of each modifier.

Id	Name	SBO
ATPc	ATP cyt.	
ADPc	ADP cyt.	

Kinetic Law

Derived unit $9.9999999999998 \cdot 10^{-10} \ mol \cdot (60 \ s)^{-1}$

$$v_{13} = \frac{\frac{\text{vol(tot_cell)}}{\text{Vt}} \cdot \text{K13} \cdot [\text{ATPc}]}{[\text{ADPc}]}$$
(39)

Table 52: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
K13	<u> </u>			$\begin{array}{c} \text{nmol} \cdot (60 \text{ s})^{-1} \cdot \\ \text{mg}^{-1} \end{array}$	

7.14 Reaction vGlyK

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

Name Glycerol kinase

Reaction equation

$$Gly3P \xrightarrow{ADPg, Gly3Pg, ATPg} Pg + Gly$$
 (40)

Reactant

Table 53: Properties of each reactant.

rable 33. I roporties of each reactant.				
Id	Name	SBO		
Gly3P	Glycerol 3-phosphate			

Modifiers

Table 54: Properties of each modifier.

Id	Name	SBO
ADPg Gly3Pg ATPg	ADP gly. Gy3P g. ATP gly.	

Products

Table 55: Properties of each product.

Id	Name	SBO
Pg Gly	Phosphates in Glycosome Glycerol	

Kinetic Law

Derived unit contains undeclared units

$$v_{14} = \frac{\frac{\text{vol(tot_cell)}}{\text{Vt}} \cdot \text{Vm}14 \cdot \left(\frac{\text{Vm}14\text{f}\cdot[\text{ADPg}]\cdot[\text{Gly}3\text{Pg}]}{\text{K}14\text{ADPg}\cdot\text{K}14\text{Gly}3\text{Pg}} - \frac{[\text{Gly}]\cdot\text{Vm}14\text{r}\cdot[\text{ATPg}]}{\text{K}14\text{ATPg}\cdot\text{K}14\text{Gly}}\right)}{\left(1 + \frac{[\text{Gly}]}{\text{K}14\text{Gly}} + \frac{[\text{Gly}3\text{Pg}]}{\text{K}14\text{Gly}3\text{Pg}}\right) \cdot \left(1 + \frac{[\text{ATPg}]}{\text{K}14\text{ATPg}} + \frac{[\text{ADPg}]}{\text{K}14\text{ADPg}}\right)}$$

$$(41)$$

Table 56: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vm14			1.00	dimensionless	\overline{Z}
Vm14r			33400.00	$nmol \cdot (60 s)^{-1} \cdot$	
				mg^{-1}	
K14ATPg			0.19	nmol $\cdot \mu l^{-1}$	
K14Gly			0.12	$nmol \cdot \mu l^{-1}$	
Vm14f			200.00	$nmol \cdot (60 s)^{-1} \cdot$	
				mg^{-1}	
K14ADPg			0.12	$nmol \cdot \mu l^{-1}$	
K14Gly3Pg			5.10	$nmol \cdot \mu l^{-1}$	\square

8 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.

8.1 Species GlcI

Name Glucose

Initial concentration $0.0340009 \text{ nmol} \cdot \mu l^{-1}$

This species takes part in two reactions (as a reactant in vHK and as a product in vGlcTr).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{GlcI} = v_1 - v_2 \tag{42}$$

8.2 Species Pg

Name Phosphates in Glycosome

Initial concentration 7.63936 nmol·µl⁻¹

This species takes part in four reactions (as a reactant in vHK, vPFK and as a product in vPGK, vGlyK).

$$\frac{\mathrm{d}}{\mathrm{d}t} Pg = v_{11} + v_{14} - v_2 - v_4 \tag{43}$$

8.3 Species Glc6P

Name Glucose 6-phosphate

Initial concentration $2.07199 \text{ nmol} \cdot \mu l^{-1}$

This species takes part in two reactions (as a reactant in vPGI and as a product in vHK).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Glc6P} = v_2 - v_3 \tag{44}$$

8.4 Species Fru6P

Name Fructose 6-phosphate

Initial concentration $0.511773 \text{ nmol} \cdot \mu l^{-1}$

This species takes part in two reactions (as a reactant in vPFK and as a product in vPGI).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Fru6P} = v_3 - v_4 \tag{45}$$

8.5 Species Fru16BP

Name Fructose 1,6-bisphosphate

Initial concentration $16.5371 \text{ nmol} \cdot \mu l^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Fru}16\mathrm{BP} = v_4 - v_5 \tag{46}$$

8.6 Species DHAP

Name Dihydroxyacetone phosphate

Initial concentration $3.89921 \text{ nmol} \cdot \mu l^{-1}$

This species takes part in four reactions (as a reactant in vTPI, vGDH and as a product in vALD, vGP0).

$$\frac{d}{dt}DHAP = v_5 + v_9 - v_6 - v_8 \tag{47}$$

8.7 Species GAP

Name Glyceraldehyde 3-phosphate

Initial concentration $0.0399329 \text{ nmol} \cdot \mu l^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{GAP} = v_5 + v_6 - v_7 \tag{48}$$

8.8 Species NAD

Name NAD

Initial concentration $3.95514 \text{ nmol} \cdot \mu l^{-1}$

This species takes part in two reactions (as a reactant in vGAPdh and as a product in vGDH).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{NAD} = v_8 - v_7 \tag{49}$$

8.9 Species BPGA13

Name 1,3-bisphosphoglycerate

Initial concentration $0.0326745 \text{ } nmol \cdot \mu l^{-1}$

This species takes part in two reactions (as a reactant in vPGK and as a product in vGAPdh).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{BPGA13} = v_7 - v_{11} \tag{50}$$

8.10 Species NADH

Name NADH

Initial concentration $0.0448639 \text{ nmol} \cdot \mu l^{-1}$

This species takes part in two reactions (as a reactant in vGDH and as a product in vGAPdh).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{NADH} = v_7 - v_8 \tag{51}$$

8.11 Species Pyr

Name Pyruvate

Initial concentration $4.77413 \text{ nmol} \cdot \mu l^{-1}$

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

$$\frac{d}{dt} Pyr = v_{12} - v_{10} \tag{52}$$

8.12 Species Nb

Name 3-PGA 2-PGA PEP

Initial concentration $1.59603 \text{ nmol} \cdot \mu l^{-1}$

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

$$\frac{d}{dt}Nb = |v_{11}| - v_{12} \tag{53}$$

8.13 Species Pc

Name Phosphates cytosol

Initial concentration $6.51839 \text{ nmol} \cdot \mu l^{-1}$

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

$$\frac{d}{dt}Pc = v_{12} - v_{13} \tag{54}$$

8.14 Species PyrE

Name Pyruvate external

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{PyrE} = 0\tag{55}$$

8.15 Species Gly

Name Glycerol

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Gly} = 0\tag{56}$$

8.16 Species GlcE

Name Glucose external

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{GlcE} = 0\tag{57}$$

8.17 Species Gly3P

Name Glycerol 3-phosphate

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

Involved in rule Gly3P

This species takes part in three reactions (as a reactant in vGPO, vGlyK and as a product in vGDH). Not these but one rule determines the species' quantity because this species is on the boundary of the reaction system.

8.18 Species ATPc

Name ATP cyt.

Involved in rule ATPc

This species takes part in two reactions (as a modifier in vPK, vATPase) and is also involved in one rule which determines this species' quantity.

8.19 Species ADPc

Name ADP cyt.

Involved in rule ADPc

This species takes part in two reactions (as a modifier in vPK, vATPase) and is also involved in one rule which determines this species' quantity.

8.20 Species ATPg

Name ATP gly.

Involved in rule ATPg

This species takes part in five reactions (as a modifier in vHK, vPFK, vALD, vPGK, vGlyK) and is also involved in one rule which determines this species' quantity.

8.21 Species ADPg

Name ADP gly.

Involved in rule ADPg

This species takes part in four reactions (as a modifier in vHK, vALD, vPGK, vGlyK) and is also involved in one rule which determines this species' quantity.

8.22 Species DHAPg

Name DHAP gly.

Involved in rule DHAPg

This species takes part in three reactions (as a modifier in vALD, vTPI, vGDH) and is also involved in one rule which determines this species' quantity.

8.23 Species DHAPc

Name DHAP cyt.

Involved in rule DHAPc

One rule which determines this species' quantity.

8.24 Species Gly3Pc

Name Gy3P c.

Involved in rule Gly3Pc

This species takes part in one reaction (as a modifier in vGPO) and is also involved in one rule which determines this species' quantity.

8.25 Species Gly3Pg

Name Gy3P g.

Involved in rule Gly3Pg

This species takes part in two reactions (as a modifier in vGDH, vGlyK) and is also involved in one rule which determines this species' quantity.

8.26 Species PGAg

Name 3-PGA g.

Involved in rule PGAg

This species takes part in one reaction (as a modifier in vPGK) and is also involved in one rule which determines this species' quantity.

8.27 Species PEPc

Name PEP c.

Involved in rule PEPc

This species takes part in one reaction (as a modifier in vPK) and is also involved in one rule which determines this species' quantity.

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