SBML Model Report

Model name: “Pritchard2002_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 two authors: Lukas Endler[1] and Pedro Mendes[2] at September 14th 2006 at 10:35 a. m. and last time modified at April eighth 2016 at 3:39 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	2
species types	0	species	25
events	0	constraints	0
reactions	19	function definitions	0
global parameters	0	unit definitions	2
rules	0	initial assignments	0

Model Notes

from:
Schemes of fluc control in a model of Saccharomyces cerevisiae glycolysis
Pritchard, L and Kell, DB Eur. J. Biochem. 269(2002), 3894-3904.
It represents a modified version of **Teusink et al.**Eur. J. Biochem. 267(2000), 5313-5329.
The model is a translation from the GEPASI file encoded by Leighton Pritchard.

[1]EMBL-EBI, lukas@ebi.ac.uk
[2]Virginia Bioinformatics Institute, mendes@vbi.vt.edu

This version uses the Vmaxes found by the best fit (R1) of Table 1 of the Pritchard and Kell paper and simulates a decrease of external glucose concentration from 100 to 2 mM.
To reproduce the values in table 2 of the publication, set GLCo to 50 mM and compute the steady state.

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 five unit definitions of which three are predefined by SBML and not mentioned in the model.

2.1 Unit `substance`

Name mmole

Definition mmol

2.2 Unit `time`

Name minute

Definition 60 s

2.3 Unit `volume`

Notes Litre is the predefined SBML unit for `volume`.

Definition l

2.4 Unit `area`

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

Definition m^2

2.5 Unit `length`

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

Definition m

3 Compartments

This model contains two compartments.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
`cell`	cytosol		3	1	litre	☑	
`ext`	exterior		3	1	litre	☑	

3.1 Compartment `cell`

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

Name cytosol

3.2 Compartment `ext`

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

Name exterior

4 Species

This model contains 25 species. The boundary condition of eight of these species is set to `true` so that these species' amount cannot be changed by any reaction. Section 6 provides further details and the derived rates of change of each species.

Table 3: Properties of each species.

Id	Name	Compartment	Derived Unit	Constant	Boundary Condition
GLCo	Glc(ext)	ext	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	☑
GLCi	Glc(int)	cell	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
ATP	ATP	cell	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
G6P	Glu6P	cell	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
ADP	ADP	cell	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
F6P	Fru6-P	cell	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
F16bP	Fru1,6-P2	cell	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
AMP	AMP	cell	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
F26bP	Fru2,6-P2	cell	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	☑
DHAP	glycerone phosphate	cell	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
GAP	Gra3P	cell	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
NAD	NAD	cell	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
BPG	Gri2,3P2	cell	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
NADH	NADH	cell	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
P3G	Gri3P	cell	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
P2G	Gri2P	cell	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
PEP	phosphoenolpyruvate	cell	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
PYR	pyruvate	cell	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
AcAld	acetaldehyde	cell	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
CO2	CO2	cell	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	☑
EtOH	ethanol	cell	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	☑

Id	Name	Compartment	Derived Unit	Constant	Boundary Condition
`Glycerol`	glycerol	`cell`	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	☑
`Glycogen`	glycogen	`cell`	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	☑
`Trehalose`	trehalose	`cell`	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	☑
`Succinate`	succinate	`cell`	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	☑

5 Reactions

This model contains 19 reactions. All reactions are listed in the following table and are subsequently described in detail. If a reaction is affected by a modifier, the identifier of this species is written above the reaction arrow.

Table 4: Overview of all reactions

№	Id	Name	Reaction Equation	SBO
1	HXT	glucose transport	$GLCo \rightleftharpoons GLCi$	
2	HK	hexokinase	$GLCi + ATP \rightleftharpoons G6P + ADP$	
3	PGI	phosphoglucose isomerase	$G6P \rightleftharpoons F6P$	
4	PFK	phosphofructosekinase	$ATP + F6P \xrightarrow{AMP,\ F26bP} ADP + F16bP$	
5	ALD	fructosebisphosphate aldolase	$F16bP \rightleftharpoons DHAP + GAP$	
6	TPI	triosephosphate isomerase	$DHAP \rightleftharpoons GAP$	
7	GAPDH	glyceraldehyde phosphate dehydrogenase	$GAP + NAD \rightleftharpoons BPG + NADH$	
8	PGK	3-phosphoglycerate kinase	$ADP + BPG \rightleftharpoons ATP + P3G$	
9	PGM	phosphoglyceromutase	$P3G \rightleftharpoons P2G$	
10	ENO	enolase	$P2G \rightleftharpoons PEP$	
11	PYK	pyruvate kinase	$ADP + PEP \rightleftharpoons ATP + PYR$	
12	PDC	pyruvate decarboxylase	$PYR \longrightarrow AcAld + CO2$	
13	ADH	alcohol dehydrogenase	$NAD + EtOH \rightleftharpoons NADH + AcAld$	
14	ATPase		$ATP \longrightarrow ADP$	
15	AK		$2\,ADP \rightleftharpoons ATP + AMP$	
16	G3PDH	glycerol-3-phosphate dehydrogenase	$DHAP + NADH \longrightarrow NAD + Glycerol$	
17	Glycogen_Branch	Glycogen_Branch	$ATP + G6P \longrightarrow ADP + Glycogen$	
18	Trehalose-_Branch	Trehalose_Branch	$ATP + 2\,G6P \longrightarrow ADP + Trehalose$	
19	Succinate-_Branch	Succinate_Branch	$3\,NAD + 2\,AcAld \longrightarrow 3\,NADH + Succinate$	

5.1 Reaction HXT

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

Name glucose transport

Reaction equation

$$\mathrm{GLCo} \rightleftharpoons \mathrm{GLCi} \tag{1}$$

Reactant

Table 5: Properties of each reactant.

Id	Name	SBO
GLCo	Glc(ext)	

Product

Table 6: Properties of each product.

Id	Name	SBO
GLCi	Glc(int)	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \frac{\frac{\mathrm{Vmax\_1} \cdot (\mathrm{[GLCo]} - \mathrm{[GLCi]})}{\mathrm{Kglc\_1}}}{1 + \frac{\mathrm{[GLCo]} + \mathrm{[GLCi]}}{\mathrm{Kglc\_1}} + \frac{\mathrm{Ki\_1} \cdot \mathrm{[GLCo]} \cdot \mathrm{[GLCi]}}{\mathrm{Kglc\_1}^2}} \tag{2}$$

Table 7: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax_1			97.240		☑
Kglc_1			1.192		☑
Ki_1			0.910		☑

5.2 Reaction HK

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

Name hexokinase

Reaction equation

$$\mathrm{GLCi} + \mathrm{ATP} \rightleftharpoons \mathrm{G6P} + \mathrm{ADP} \tag{3}$$

Reactants

Table 8: Properties of each reactant.

Id	Name	SBO
GLCi	Glc(int)	
ATP	ATP	

Products

Table 9: Properties of each product.

Id	Name	SBO
G6P	Glu6P	
ADP	ADP	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \frac{\mathrm{vol}\,(\mathrm{cell}) \cdot \mathrm{Vmax\_2} \cdot \left(\frac{[\mathrm{GLCi}] \cdot [\mathrm{ATP}]}{\mathrm{Kglc\_2} \cdot \mathrm{Katp\_2}} - \frac{[\mathrm{G6P}] \cdot [\mathrm{ADP}]}{\mathrm{Kglc\_2} \cdot \mathrm{Katp\_2} \cdot \mathrm{Keq\_2}} \right)}{\left(1 + \frac{[\mathrm{GLCi}]}{\mathrm{Kglc\_2}} + \frac{[\mathrm{G6P}]}{\mathrm{Kg6p\_2}}\right) \cdot \left(1 + \frac{[\mathrm{ATP}]}{\mathrm{Katp\_2}} + \frac{[\mathrm{ADP}]}{\mathrm{Kadp\_2}}\right)} \tag{4}$$

Table 10: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax_2			236.70		☑
Kglc_2			0.08		☑
Katp_2			0.15		☑
Keq_2			2000.00		☑
Kg6p_2			30.00		☑
Kadp_2			0.23		☑

5.3 Reaction PGI

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

Name phosphoglucose isomerase

Reaction equation

$$\mathrm{G6P} \rightleftharpoons \mathrm{F6P} \tag{5}$$

Reactant

Table 11: Properties of each reactant.

Id	Name	SBO
G6P	Glu6P	

Product

Table 12: Properties of each product.

Id	Name	SBO
F6P	Fru6-P	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \frac{\mathrm{vol}\,(\mathrm{cell}) \cdot \mathrm{Vmax\_3} \cdot \left(\frac{[\mathrm{G6P}]}{\mathrm{Kg6p\_3}} - \frac{[\mathrm{F6P}]}{\mathrm{Kg6p\_3} \cdot \mathrm{Keq\_3}} \right)}{1 + \frac{[\mathrm{G6P}]}{\mathrm{Kg6p\_3}} + \frac{[\mathrm{F6P}]}{\mathrm{Kf6p\_3}}} \tag{6}$$

Table 13: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax_3			1056.00		☑
Kg6p_3			1.40		☑
Keq_3			0.29		☑
Kf6p_3			0.30		☑

5.4 Reaction PFK

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

Name phosphofructosekinase

Reaction equation

$$\mathrm{ATP} + \mathrm{F6P} \xrightarrow{\mathrm{AMP,\ F26bP}} \mathrm{ADP} + \mathrm{F16bP} \tag{7}$$

Reactants

Table 14: Properties of each reactant.

Id	Name	SBO
ATP	ATP	
F6P	Fru6-P	

Modifiers

Table 15: Properties of each modifier.

Id	Name	SBO
AMP	AMP	
F26bP	Fru2,6-P2	

Products

Table 16: Properties of each product.

Id	Name	SBO
ADP	ADP	
F16bP	Fru1,6-P2	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \mathrm{vol}\,(\mathrm{cell}) \cdot \mathrm{Vmax\_4} \cdot \frac{\mathrm{gR\_4} \cdot \frac{[\mathrm{F6P}]}{\mathrm{Kf6p\_4}} \cdot \frac{[\mathrm{ATP}]}{\mathrm{Katp\_4}} \cdot \left(1 + \frac{[\mathrm{F6P}]}{\mathrm{Kf6p\_4}} + \frac{[\mathrm{ATP}]}{\mathrm{Katp\_4}} + \frac{\frac{\mathrm{gR\_4} \cdot [\mathrm{F6P}]}{\mathrm{Kf6p\_4}} \cdot [\mathrm{ATP}]}{\mathrm{Katp\_4}}\right)}{\left(1 + \frac{[\mathrm{F6P}]}{\mathrm{Kf6p\_4}} + \frac{[\mathrm{ATP}]}{\mathrm{Katp\_4}} + \frac{\frac{\mathrm{gR\_4} \cdot [\mathrm{F6P}]}{\mathrm{Kf6p\_4}} \cdot [\mathrm{ATP}]}{\mathrm{Katp\_4}}\right)^2 + \mathrm{L0\_4} \cdot \left(\frac{1 + \frac{\mathrm{Ciatp\_4} \cdot [\mathrm{ATP}]}{\mathrm{Kiatp\_4}}}{1 + \frac{[\mathrm{ATP}]}{\mathrm{Kiatp\_4}}}\right)^2 \cdot \left(\frac{1 + \frac{\mathrm{Camp\_4} \cdot [\mathrm{AMP}]}{\mathrm{Kamp\_4}}}{1 + \frac{[\mathrm{AMP}]}{\mathrm{Kamp\_4}}}\right)^2 \cdot \left(\frac{1 + \frac{\mathrm{Cf26\_4} \cdot [\mathrm{F26bP}]}{\mathrm{Kf26\_4}} + \frac{\mathrm{Cf16\_4} \cdot [\mathrm{F16bP}]}{\mathrm{Kf16\_4}}}{1 + \frac{[\mathrm{F26bP}]}{\mathrm{Kf26\_4}} + \frac{[\mathrm{F16bP}]}{\mathrm{Kf16\_4}}}\right)^2} \tag{8}$$

Table 17: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax_4			110.000		☑
gR_4			5.120		☑
Kf6p_4			0.100		☑
Katp_4			0.710		☑
L0_4			0.660		☑
Ciatp_4			100.000		☑
Kiatp_4			0.650		☑
Camp_4			0.085		☑
Kamp_4			0.100		☑
Cf26_4			0.017		☑
Kf26_4			$6.82 \cdot 10^{-4}$		☑
Cf16_4			0.397		☑
Kf16_4			0.111		☑
Catp_4			3.000		☑

5.5 Reaction ALD

This is a reversible reaction of one reactant forming two products.

Name fructosebisphosphate aldolase

Reaction equation

$$\mathrm{F16bP} \rightleftharpoons \mathrm{DHAP} + \mathrm{GAP} \tag{9}$$

Reactant

Table 18: Properties of each reactant.

Id	Name	SBO
F16bP	Fru1,6-P2	

Products

Table 19: Properties of each product.

Id	Name	SBO
DHAP	glycerone phosphate	
GAP	Gra3P	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \frac{\mathrm{vol}\,(\mathrm{cell}) \cdot \mathrm{Vmax\_5} \cdot \left(\frac{[\mathrm{F16bP}]}{\mathrm{Kf16bp\_5}} - \frac{[\mathrm{DHAP}] \cdot [\mathrm{GAP}]}{\mathrm{Kf16bp\_5} \cdot \mathrm{Keq\_5}} \right)}{1 + \frac{[\mathrm{F16bP}]}{\mathrm{Kf16bp\_5}} + \frac{[\mathrm{DHAP}]}{\mathrm{Kdhap\_5}} + \frac{[\mathrm{GAP}]}{\mathrm{Kgap\_5}} + \frac{[\mathrm{F16bP}] \cdot [\mathrm{GAP}]}{\mathrm{Kf16bp\_5} \cdot \mathrm{Kigap\_5}} + \frac{[\mathrm{DHAP}] \cdot [\mathrm{GAP}]}{\mathrm{Kdhap\_5} \cdot \mathrm{Kgap\_5}}} \tag{10}$$

Table 20: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax_5			94.690		☑
Kf16bp_5			0.300		☑
Keq_5			0.069		☑
Kdhap_5			2.000		☑
Kgap_5			2.400		☑
Kigap_5			10.000		☑

5.6 Reaction TPI

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

Name triosephosphate isomerase

Reaction equation

$$\mathrm{DHAP} \rightleftharpoons \mathrm{GAP} \tag{11}$$

Reactant

Table 21: Properties of each reactant.

Id	Name	SBO
DHAP	glycerone phosphate	

Product

Table 22: Properties of each product.

Id	Name	SBO
GAP	Gra3P	

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \mathrm{vol}\,(\mathrm{cell}) \cdot (\mathrm{k1\_6} \cdot [\mathrm{DHAP}] - \mathrm{k2\_6} \cdot [\mathrm{GAP}]) \tag{12}$$

Table 23: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1_6			450000.000		☑
k2_6			10^7		☑

5.7 Reaction GAPDH

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

Name glyceraldehyde phosphate dehydrogenase

Reaction equation

$$\mathrm{GAP} + \mathrm{NAD} \rightleftharpoons \mathrm{BPG} + \mathrm{NADH} \tag{13}$$

Reactants

Table 24: Properties of each reactant.

Id	Name	SBO
GAP	Gra3P	
NAD	NAD	

Products

Table 25: Properties of each product.

Id	Name	SBO
BPG	Gri2,3P2	
NADH	NADH	

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \frac{\mathrm{vol}\,(\mathrm{cell}) \cdot \mathrm{C\_7} \cdot \left(\frac{\mathrm{Vmaxf\_7} \cdot [\mathrm{GAP}] \cdot [\mathrm{NAD}]}{\mathrm{Kgap\_7} \cdot \mathrm{Knad\_7}} - \frac{\mathrm{Vmaxr\_7} \cdot [\mathrm{BPG}] \cdot [\mathrm{NADH}]}{\mathrm{Kbpg\_7} \cdot \mathrm{Knadh\_7}} \right)}{\left(1 + \frac{[\mathrm{GAP}]}{\mathrm{Kgap\_7}} + \frac{[\mathrm{BPG}]}{\mathrm{Kbpg\_7}}\right) \cdot \left(1 + \frac{[\mathrm{NAD}]}{\mathrm{Knad\_7}} + \frac{[\mathrm{NADH}]}{\mathrm{Knadh\_7}}\right)} \tag{14}$$

Table 26: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
C_7			1.000		☑
Vmaxf_7			1152.000		☑
Kgap_7			0.210		☑
Knad_7			0.090		☑
Vmaxr_7			6719.000		☑
Kbpg_7			0.010		☑
Knadh_7			0.060		☑

5.8 Reaction PGK

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

Name 3-phosphoglycerate kinase

Reaction equation

$$\mathrm{ADP} + \mathrm{BPG} \rightleftharpoons \mathrm{ATP} + \mathrm{P3G} \tag{15}$$

Reactants

Table 27: Properties of each reactant.

Id	Name	SBO
ADP	ADP	
BPG	Gri2,3P2	

Products

Table 28: Properties of each product.

Id	Name	SBO
ATP	ATP	
P3G	Gri3P	

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \frac{\mathrm{vol}\,(\mathrm{cell}) \cdot \mathrm{Vmax\_8} \cdot \frac{\mathrm{Keq\_8}\cdot[\mathrm{BPG}]\cdot[\mathrm{ADP}]-[\mathrm{P3G}]\cdot[\mathrm{ATP}]}{\mathrm{Kp3g\_8}\cdot\mathrm{Katp\_8}}}{\left(1+\frac{[\mathrm{BPG}]}{\mathrm{Kbpg\_8}}+\frac{[\mathrm{P3G}]}{\mathrm{Kp3g\_8}}\right)\cdot\left(1+\frac{[\mathrm{ADP}]}{\mathrm{Kadp\_8}}+\frac{[\mathrm{ATP}]}{\mathrm{Katp\_8}}\right)} \tag{16}$$

Table 29: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax_8			1288.000		☑
Keq_8			3200.000		☑
Kp3g_8			0.530		☑
Katp_8			0.300		☑
Kbpg_8			0.003		☑
Kadp_8			0.200		☑

5.9 Reaction PGM

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

Name phosphoglyceromutase

Reaction equation

$$\mathrm{P3G} \rightleftharpoons \mathrm{P2G} \tag{17}$$

Reactant

Table 30: Properties of each reactant.

Id	Name	SBO
P3G	Gri3P	

Product

Table 31: Properties of each product.

Id	Name	SBO
P2G	Gri2P	

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \frac{\mathrm{vol}\,(\mathrm{cell}) \cdot \mathrm{Vmax\_9} \cdot \left(\frac{[\mathrm{P3G}]}{\mathrm{Kp3g\_9}} - \frac{[\mathrm{P2G}]}{\mathrm{Kp3g\_9} \cdot \mathrm{Keq\_9}} \right)}{1 + \frac{[\mathrm{P3G}]}{\mathrm{Kp3g\_9}} + \frac{[\mathrm{P2G}]}{\mathrm{Kp2g\_9}}} \tag{18}$$

Table 32: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax_9			2585.00		☑
Kp3g_9			1.20		☑
Keq_9			0.19		☑
Kp2g_9			0.08		☑

5.10 Reaction ENO

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

Name enolase

Reaction equation

$$\mathrm{P2G} \rightleftharpoons \mathrm{PEP} \tag{19}$$

Reactant

Table 33: Properties of each reactant.

Id	Name	SBO
P2G	Gri2P	

Product

Table 34: Properties of each product.

Id	Name	SBO
PEP	phosphoenolpyruvate	

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = \frac{\mathrm{vol}\,(\mathrm{cell}) \cdot \mathrm{Vmax\_10} \cdot \left(\frac{[\mathrm{P2G}]}{\mathrm{Kp2g\_10}} - \frac{[\mathrm{PEP}]}{\mathrm{Kp2g\_10} \cdot \mathrm{Keq\_10}} \right)}{1 + \frac{[\mathrm{P2G}]}{\mathrm{Kp2g\_10}} + \frac{[\mathrm{PEP}]}{\mathrm{Kpep\_10}}} \tag{20}$$

Table 35: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax_10			201.60		☑
Kp2g_10			0.04		☑
Keq_10			6.70		☑
Kpep_10			0.50		☑

5.11 Reaction PYK

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

Name pyruvate kinase

Reaction equation

$$\mathrm{ADP} + \mathrm{PEP} \rightleftharpoons \mathrm{ATP} + \mathrm{PYR} \tag{21}$$

Reactants

Table 36: Properties of each reactant.

Id	Name	SBO
ADP	ADP	
PEP	phosphoenolpyruvate	

Products

Table 37: Properties of each product.

Id	Name	SBO
ATP	ATP	
PYR	pyruvate	

Kinetic Law

Derived unit contains undeclared units

$$v_{11} = \frac{\mathrm{vol}\,(\mathrm{cell}) \cdot \mathrm{Vmax\_11} \cdot \left(\frac{[\mathrm{PEP}] \cdot [\mathrm{ADP}]}{\mathrm{Kpep\_11} \cdot \mathrm{Kadp\_11}} - \frac{[\mathrm{PYR}] \cdot [\mathrm{ATP}]}{\mathrm{Kpep\_11} \cdot \mathrm{Kadp\_11} \cdot \mathrm{Keq\_11}} \right)}{\left(1 + \frac{[\mathrm{PEP}]}{\mathrm{Kpep\_11}} + \frac{[\mathrm{PYR}]}{\mathrm{Kpyr\_11}} \right) \cdot \left(1 + \frac{[\mathrm{ADP}]}{\mathrm{Kadp\_11}} + \frac{[\mathrm{ATP}]}{\mathrm{Katp\_11}} \right)} \tag{22}$$

Table 38: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax_11			1000.00		☑
Kpep_11			0.14		☑
Kadp_11			0.53		☑
Keq_11			6500.00		☑
Kpyr_11			21.00		☑
Katp_11			1.50		☑

5.12 Reaction PDC

This is an irreversible reaction of one reactant forming two products.

Name pyruvate decarboxylase

Reaction equation

$$\mathrm{PYR} \longrightarrow \mathrm{AcAld} + \mathrm{CO2} \tag{23}$$

Reactant

Table 39: Properties of each reactant.

Id	Name	SBO
PYR	pyruvate	

Id	Name	SBO

Products

Table 40: Properties of each product.

Id	Name	SBO
AcAld	acetaldehyde	
CO2	CO2	

Kinetic Law

Derived unit contains undeclared units

$$v_{12} = \frac{\mathrm{vol}\,(\mathrm{cell}) \cdot \mathrm{Vmax\_12} \cdot \left(\frac{[\mathrm{PYR}]}{\mathrm{Kpyr\_12}}\right)^{\mathrm{nH\_12}}}{1 + \left(\frac{[\mathrm{PYR}]}{\mathrm{Kpyr\_12}}\right)^{\mathrm{nH\_12}}} \tag{24}$$

Table 41: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax_12			857.80		☑
Kpyr_12			4.33		☑
nH_12			1.90		☑

5.13 Reaction ADH

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

Name alcohol dehydrogenase

Reaction equation

$$\mathrm{NAD} + \mathrm{EtOH} \rightleftharpoons \mathrm{NADH} + \mathrm{AcAld} \tag{25}$$

Reactants

Table 42: Properties of each reactant.

Id	Name	SBO
NAD	NAD	
EtOH	ethanol	

Products

Table 43: Properties of each product.

Id	Name	SBO
NADH	NADH	
AcAld	acetaldehyde	

Kinetic Law

Derived unit contains undeclared units

$$v_{13} = \frac{\text{vol}(\text{cell}) \cdot \text{Vmax\_13} \cdot \left(\frac{[\text{EtOH}] \cdot [\text{NAD}]}{\text{Ketoh\_13} \cdot \text{Kinad\_13}} - \text{I} \right.}{1 + \frac{[\text{NAD}]}{\text{Kinad\_13}} + \frac{[\text{EtOH}] \cdot \text{Knad\_13}}{\text{Kinad\_13} \cdot \text{Ketoh\_13}} + \frac{[\text{AcAld}] \cdot \text{Knadh\_13}}{\text{Kinadh\_13} \cdot \text{Kacald\_13}} + \frac{[\text{NADH}]}{\text{Kinadh\_13}} + \frac{[\text{EtOH}] \cdot [\text{NAD}]}{\text{Kinad\_13} \cdot \text{Ketoh\_13}} + \frac{[\text{NAD}] \cdot [\text{AcAld}] \cdot \text{Knadh\_13}}{\text{Kinad\_13} \cdot \text{Kinadh\_13} \cdot \text{Kacald\_13}} + \frac{[\text{Et}}{\text{Kinac}}} \tag{26}$$

Table 44: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax_13			209.500		☑
Ketoh_13			17.000		☑
Kinad_13			0.920		☑
Keq_13			$6.9 \cdot 10^{-5}$		☑
Knad_13			0.170		☑
Knadh_13			0.110		☑
Kinadh_13			0.031		☑
Kacald_13			1.110		☑
Kiacald_13			1.100		☑
Kietoh_13			90.000		☑

5.14 Reaction ATPase

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

Reaction equation

$$\mathrm{ATP} \longrightarrow \mathrm{ADP} \tag{27}$$

Reactant

Table 45: Properties of each reactant.

Id	Name	SBO
ATP	ATP	

Product

Table 46: Properties of each product.

Id	Name	SBO
ADP	ADP	

Kinetic Law

Derived unit contains undeclared units

$$v_{14} = \mathrm{vol}\,(\mathrm{cell}) \cdot \mathrm{Katpase\_14} \cdot [\mathrm{ATP}] \tag{28}$$

Table 47: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Katpase_14			39.5		☑

5.15 Reaction AK

This is a reversible reaction of one reactant forming two products.

Reaction equation

$$2\,\mathrm{ADP} \rightleftharpoons \mathrm{ATP} + \mathrm{AMP} \tag{29}$$

Reactant

Table 48: Properties of each reactant.

Id	Name	SBO
ADP	ADP	

Products

Table 49: Properties of each product.

Id	Name	SBO
ATP	ATP	
AMP	AMP	

Kinetic Law

Derived unit contains undeclared units

$$v_{15} = \mathrm{vol}\,(\mathrm{cell}) \cdot (\mathrm{k1\_15} \cdot [\mathrm{ADP}] \cdot [\mathrm{ADP}] - \mathrm{k2\_15} \cdot [\mathrm{ATP}] \cdot [\mathrm{AMP}]) \tag{30}$$

Table 50: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1_15			45.0		☑
k2_15			100.0		☑

5.16 Reaction G3PDH

This is an irreversible reaction of two reactants forming two products.

Name glycerol-3-phosphate dehydrogenase

Reaction equation

$$\mathrm{DHAP} + \mathrm{NADH} \longrightarrow \mathrm{NAD} + \mathrm{Glycerol} \tag{31}$$

Reactants

Table 51: Properties of each reactant.

Id	Name	SBO
DHAP	glycerone phosphate	

Id	Name	SBO
NADH	NADH	

Products

Table 52: Properties of each product.

Id	Name	SBO
NAD	NAD	
Glycerol	glycerol	

Kinetic Law

Derived unit contains undeclared units

$$v_{16} = \frac{\mathrm{vol}\,(\mathrm{cell}) \cdot \mathrm{Vmax\_16} \cdot \left(\frac{[\mathrm{DHAP}]}{\mathrm{Kdhap\_16}} \cdot \frac{[\mathrm{NADH}]}{\mathrm{Knadh\_16}} - \frac{[\mathrm{Glycerol}]}{\mathrm{Kdhap\_16}} \cdot \frac{[\mathrm{NAD}]}{\mathrm{Knadh\_16}} \cdot \frac{1}{\mathrm{Keq\_16}} \right)}{\left(1 + \frac{[\mathrm{DHAP}]}{\mathrm{Kdhap\_16}} + \frac{[\mathrm{Glycerol}]}{\mathrm{Kglycerol\_16}} \right) \cdot \left(1 + \frac{[\mathrm{NADH}]}{\mathrm{Knadh\_16}} + \frac{[\mathrm{NAD}]}{\mathrm{Knad\_16}} \right)} \tag{32}$$

Table 53: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax_16			47.110		☑
Kdhap_16			0.400		☑
Knadh_16			0.023		☑
Keq_16			4300.000		☑
Kglycerol_16			1.000		☑
Knad_16			0.930		☑

5.17 Reaction Glycogen_Branch

This is an irreversible reaction of two reactants forming two products.

Name Glycogen_Branch

Reaction equation

$$\mathrm{ATP} + \mathrm{G6P} \longrightarrow \mathrm{ADP} + \mathrm{Glycogen} \tag{33}$$

Reactants

Table 54: Properties of each reactant.

Id	Name	SBO
ATP	ATP	
G6P	Glu6P	

Products

Table 55: Properties of each product.

Id	Name	SBO
ADP	ADP	
Glycogen	glycogen	

Kinetic Law

Derived unit contains undeclared units

$$v_{17} = \mathrm{vol}\,(\mathrm{cell}) \cdot \mathrm{KGLYCOGEN\_17} \tag{34}$$

Table 56: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
KGLYCOGEN_17			6.0		☑

5.18 Reaction Trehalose_Branch

This is an irreversible reaction of two reactants forming two products.

Name Trehalose_Branch

Reaction equation

$$\mathrm{ATP} + 2\,\mathrm{G6P} \longrightarrow \mathrm{ADP} + \mathrm{Trehalose} \tag{35}$$

Reactants

Table 57: Properties of each reactant.

Id	Name	SBO
ATP	ATP	

Id	Name	SBO
G6P	Glu6P	

Products

Table 58: Properties of each product.

Id	Name	SBO
ADP	ADP	
Trehalose	trehalose	

Kinetic Law

Derived unit contains undeclared units

$$v_{18} = \mathrm{vol}\,(\mathrm{cell}) \cdot \mathrm{Ktrehalose\_18} \tag{36}$$

Table 59: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Ktrehalose_18			2.4		☑

5.19 Reaction Succinate_Branch

This is an irreversible reaction of two reactants forming two products.

Name Succinate_Branch

Reaction equation

$$3\,\mathrm{NAD} + 2\,\mathrm{AcAld} \longrightarrow 3\,\mathrm{NADH} + \mathrm{Succinate} \tag{37}$$

Reactants

Table 60: Properties of each reactant.

Id	Name	SBO
NAD	NAD	
AcAld	acetaldehyde	

Products

Table 61: Properties of each product.

Id	Name	SBO
NADH	NADH	
Succinate	succinate	

Kinetic Law

Derived unit contains undeclared units

$$v_{19} = \mathrm{vol}\,(\mathrm{cell}) \cdot \mathrm{k\_19} \cdot [\mathrm{AcAld}] \tag{38}$$

Table 62: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k_19			21.4		☑

6 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.

6.1 Species GLCo

Name Glc(ext)

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{GLCo} = 0 \tag{39}$$

6.2 Species GLCi

Name Glc(int)

Initial concentration $0.097652231064563\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in HK and as a product in HXT).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{GLCi} = v_1 - v_2 \tag{40}$$

6.3 Species ATP

Name ATP

Initial concentration $2.52512746499271\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in eight reactions (as a reactant in HK, PFK, ATPase, Glycogen_Branch, Trehalose_Branch and as a product in PGK, PYK, AK).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ATP} = v_8 + v_{11} + v_{15} - v_2 - v_4 - v_{14} - v_{17} - v_{18} \tag{41}$$

6.4 Species G6P

Name Glu6P

Initial concentration $2.67504014044787\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in four reactions (as a reactant in PGI, Glycogen_Branch, Trehalose_Branch and as a product in HK).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{G6P} = v_2 - v_3 - v_{17} - 2\,v_{18} \tag{42}$$

6.5 Species ADP

Name ADP

Initial concentration $1.28198768168719\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in eight reactions (as a reactant in PGK, PYK, AK and as a product in HK, PFK, ATPase, Glycogen_Branch, Trehalose_Branch).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ADP} = v_2 + v_4 + v_{14} + v_{17} + v_{18} - v_8 - v_{11} - 2\,v_{15} \tag{43}$$

6.6 Species F6P

Name Fru6-P

Initial concentration 0.624976405532373 mmol · l^{-1}

This species takes part in two reactions (as a reactant in PFK and as a product in PGI).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{F6P} = v_3 - v_4 \tag{44}$$

6.7 Species F16bP

Name Fru1,6-P2

Initial concentration 6.22132076069411 mmol · l^{-1}

This species takes part in two reactions (as a reactant in ALD and as a product in PFK).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{F16bP} = v_4 - v_5 \tag{45}$$

6.8 Species AMP

Name AMP

Initial concentration 0.292884853320091 mmol · l^{-1}

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{AMP} = v_{15} \tag{46}$$

6.9 Species F26bP

Name Fru2,6-P2

Initial concentration 0.02 mmol · l^{-1}

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{F26bP} = 0 \tag{47}$$

6.10 Species DHAP

Name glycerone phosphate

Initial concentration 1.00415254899644 mmol · l^{-1}

This species takes part in three reactions (as a reactant in TPI, G3PDH and as a product in ALD).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{DHAP} = v_5 - v_6 - v_{16} \tag{48}$$

6.11 Species GAP

Name Gra3P

Initial concentration $0.0451809175780963\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in three reactions (as a reactant in GAPDH and as a product in ALD, TPI).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{GAP} = v_5 + v_6 - v_7 \tag{49}$$

6.12 Species NAD

Name NAD

Initial concentration $1.50329030201531\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in four reactions (as a reactant in GAPDH, ADH, Succinate_Branch and as a product in G3PDH).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{NAD} = v_{16} - v_7 - v_{13} - 3\,v_{19} \tag{50}$$

6.13 Species BPG

Name Gri2,3P2

Initial concentration $7.36873499865602\cdot 10^{-4}\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in PGK and as a product in GAPDH).

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

6.14 Species NADH

Name NADH

Initial concentration $0.0867096979846952\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in four reactions (as a reactant in G3PDH and as a product in GAPDH, ADH, Succinate_Branch).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{NADH} = v_7 + v_{13} + 3\,v_{19} - v_{16} \tag{52}$$

6.15 Species P3G

Name Gri3P

Initial concentration $0.885688538360659\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in PGM and as a product in PGK).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{P3G} = v_8 - v_9 \tag{53}$$

6.16 Species P2G

Name Gri2P

Initial concentration $0.127695817386632\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in ENO and as a product in PGM).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{P2G} = v_9 - v_{10} \tag{54}$$

6.17 Species PEP

Name phosphoenolpyruvate

Initial concentration $0.0632352144936527\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in PYK and as a product in ENO).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{PEP} = v_{10} - v_{11} \tag{55}$$

6.18 Species PYR

Name pyruvate

Initial concentration $1.81531251192736\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in PDC and as a product in PYK).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{PYR} = v_{11} - v_{12} \tag{56}$$

6.19 Species AcAld

Name acetaldehyde

Initial concentration $0.178140579850657\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in three reactions (as a reactant in Succinate_Branch and as a product in PDC, ADH).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{AcAld} = v_{12} + v_{13} - 2\,v_{19} \tag{57}$$

6.20 Species CO2

Name CO2

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{CO2} = 0 \tag{58}$$

6.21 Species EtOH

Name ethanol

Initial concentration $50\ \mathrm{mmol} \cdot \mathrm{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{EtOH} = 0 \tag{59}$$

6.22 Species Glycerol

Name glycerol

Initial concentration $0.15\ \mathrm{mmol} \cdot \mathrm{l}^{-1}$

This species takes part in one reaction (as a product in G3PDH), which does not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Glycerol} = 0 \tag{60}$$

6.23 Species Glycogen

Name glycogen

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Glycogen} = 0 \tag{61}$$

6.24 Species Trehalose

Name trehalose

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Trehalose} = 0 \tag{62}$$

6.25 Species Succinate

Name succinate

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Succinate} = 0 \tag{63}$$

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

[a]Center for Bioinformatics Tübingen (ZBIT), Germany
[b]California Institute of Technology, Beckman Institute BNMC, Pasadena, United States
[c]European Bioinformatics Institute, Wellcome Trust Genome Campus, Hinxton, United Kingdom
[d]EML Research gGmbH, Heidelberg, Germany