SBML Model Report

Model name: “Albert2005_Glycolysis”

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1 General Overview

This is a document in SBML Level 2 Version 3 format. This model was created by the following three authors: Vijayalakshmi Chelliah[1], Marvin Schulz[2] and Paul A. M. Michels[3] at January 27th 2009 at 2:07 p. m. and last time modified at April eighth 2016 at 4:01 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	3
species types	0	species	27
events	0	constraints	0
reactions	21	function definitions	13
global parameters	5	unit definitions	3
rules	0	initial assignments	0

Model Notes

This model is from the article:
Experimental and in silico analyses of glycolytic flux control in bloodstream form Trypanosoma brucei.
Albert MA, Haanstra JR, Hannaert V, Van Roy J, Opperdoes FR, Bakker BM, Michels PA. J

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Abstract:
A mathematical model of glycolysis in bloodstream form Trypanosoma brucei was developed previously on the basis of all available enzyme kinetic data (Bakker, B. M., Michels, P. A. M., Opperdoes, F. R., and Westerhoff, H. V. (1997) J. Biol. Chem. 272, 3207-3215). The model predicted correctly the fluxes and cellular metabolite concentrations as measured in non-growing trypanosomes and the major contribution to the flux control exerted by the plasma membrane glucose transporter. Surprisingly, a large overcapacity was predicted for hexokinase (HXK), phosphofructokinase (PFK), and pyruvate kinase (PYK). Here, we present our further analysis of the control of glycolytic flux in bloodstream form T. brucei. First, the model was optimized and extended with recent information about the kinetics of enzymes and their activities as measured in lysates of in vitro cultured growing trypanosomes. Second, the concentrations of five glycolytic enzymes (HXK, PFK, phosphoglycerate mutase, enolase, and PYK) in trypanosomes were changed by RNA interference. The effects of the knockdown of these enzymes on the growth, activities, and levels of various enzymes and glycolytic flux were studied and compared with model predictions. Data thus obtained support the conclusion from the in silico analysis that HXK, PFK, and PYK are in excess, albeit less than predicted. Interestingly, depletion of PFK and enolase had an effect on the activity (but not, or to a lesser extent, expression) of some other glycolytic enzymes. Enzymes located both in the glycosomes (the peroxisome-like organelles harboring the first seven enzymes of the glycolytic pathway of trypanosomes) and in the cytosol were affected. These data suggest the existence of novel regulatory mechanisms operating in trypanosome glycolysis.

2 Unit Definitions

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

2.1 Unit `time`

Definition s

2.2 Unit `substance`

Definition mmol

2.3 Unit `volume`

Definition ml

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 three compartments.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
`compartment_1`	cytosol		3	1	litre	☑	
`compartment_2`	glycosome		3	1	litre	☑	
`compartment_3`	extracellular		3	1	litre	☑	

3.1 Compartment `compartment_1`

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

Name cytosol

3.2 Compartment `compartment_2`

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

Name glycosome

3.3 Compartment `compartment_3`

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

Name extracellular

4 Species

This model contains 27 species. The boundary condition of three 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 Condition
species_1	pyruvate	compartment_1	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	⊟	⊟
species_2	adpc	compartment_1	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	⊟	⊟
species_3	atpc	compartment_1	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	⊟	⊟
species_4	phosphoenolpyruvate	compartment_1	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	⊟	⊟
species_5	2phosphoglycerate	compartment_1	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	⊟	⊟
species_6	ampc	compartment_1	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	⊟	⊟
species_7	3phosphoglycerate cytosol	compartment_1	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	⊟	⊟
species_8	dihydroxyacetonephosphate cytosol	compartment_1	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	⊟	⊟
species_9	glycerol3phosphate cytosol	compartment_1	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	⊟	⊟
species_10	glucose	compartment_2	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	⊟	⊟
species_11	atpg	compartment_2	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	⊟	⊟
species_12	adpg	compartment_2	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	⊟	⊟
species_13	ampg	compartment_2	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	⊟	⊟
species_14	glucose6phosphate	compartment_2	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	⊟	⊟
species_15	fructose6phosphate	compartment_2	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	⊟	⊟
species_16	fructose16bisphosphate	compartment_2	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	⊟	⊟
species_17	dihydroxyacetonephosphate	compartment_2	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	⊟	⊟
species_18	glyceraldehyde3phosphate	compartment_2	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	⊟	⊟
species_19	nad	compartment_2	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	⊟	⊟
species_20	nadh	compartment_2	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	⊟	⊟
species_21	bisphosphoglycerate	compartment_2	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	⊟	⊟

Id	Name	Compartment	Derived Unit	Constant	Boundary Condition
`species_22`	glycerol3phosphate	`compartment_2`	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	$\boxminus$	$\boxminus$
`species_23`	3phosphoglycerate	`compartment_2`	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	$\boxminus$	$\boxminus$
`species_24`	glycerol	`compartment_2`	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	$\boxminus$	$\boxminus$
`species_25`	glucose external	`compartment_3`	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	☑	☑
`species_26`	pyruvate external	`compartment_3`	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	☑	☑
`species_27`	glycerol external	`compartment_3`	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	☑	☑

5 Parameters

This model contains five global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
RaHXK	RaHXK		1.0		☑
RaPFK	RaPFK		1.0		☑
RaPYK	RaPYK		1.0		☑
RaPGAM	RaPGAM		1.0		☑
RaENO	RaENO		1.0		☑

6 Function definitions

This is an overview of 13 function definitions.

6.1 Function definition function_17

Name Henri-Michaelis-Menten (irreversible)

Arguments substrate, Km, V

Mathematical Expression

$$\frac{\mathrm{V} \cdot \mathrm{substrate}}{\mathrm{Km} + \mathrm{substrate}} \tag{1}$$

6.2 Function definition function_12

Name Reversible Michaelis-Menten

Arguments substrate, product, Kms, Kmp, Vf, Vr

Mathematical Expression

$$\frac{\frac{\mathrm{Vf} \cdot \mathrm{substrate}}{\mathrm{Kms}} - \frac{\mathrm{Vr} \cdot \mathrm{product}}{\mathrm{Kmp}}}{1 + \frac{\mathrm{substrate}}{\mathrm{Kms}} + \frac{\mathrm{product}}{\mathrm{Kmp}}} \tag{2}$$

6.3 Function definition function_15

Name Rate Law for glyceraldehyde3phosphatedehydrogenase

Arguments Vmax_v7, GAP, KGAP_v7, NAD, KNAD_v7, r_v7, BPGA13, KBPGA13_v7, NADH, KNADH_v7

Mathematical Expression

$$\mathrm{Vmax\_v7} \cdot \frac{\frac{\mathrm{GAP}}{\mathrm{KGAP\_v7}} \cdot \frac{\mathrm{NAD}}{\mathrm{KNAD\_v7}} - \mathrm{r\_v7} \cdot \frac{\mathrm{BPGA13}}{\mathrm{KBPGA13\_v7}} \cdot \frac{\mathrm{NADH}}{\mathrm{KNADH\_v7}}}{\left(1 + \frac{\mathrm{GAP}}{\mathrm{KGAP\_v7}} + \frac{\mathrm{BPGA13}}{\mathrm{KBPGA13\_v7}}\right) \cdot \left(1 + \frac{\mathrm{NAD}}{\mathrm{KNAD\_v7}} + \frac{\mathrm{NADH}}{\mathrm{KNADH\_v7}}\right)} \tag{3}$$

6.4 Function definition function_20

Name Rate Law for atp utilisation

Arguments k, atpc, adpc

Mathematical Expression

$$\frac{\mathrm{k} \cdot \mathrm{atpc}}{\mathrm{adpc}} \tag{4}$$

6.5 Function definition function_19

Name Rate Law for pyruvate kinase

Arguments Vmax_v12, PEP, PK_n, ADPc, KADP_v12, ATPc

Mathematical Expression

$$\frac{\mathrm{Vmax\_v12} \cdot \left(\frac{\mathrm{PEP}}{0.34 \cdot \left(1 + \frac{\mathrm{ATPc}}{0.57} + \frac{\mathrm{ADPc}}{0.64}\right)}\right)^{\mathrm{PK\_n}} \cdot \frac{\mathrm{ADPc}}{\mathrm{KADP\_v12}}}{\left(1 + \left(\frac{\mathrm{PEP}}{0.34 \cdot \left(1 + \frac{\mathrm{ATPc}}{0.57} + \frac{\mathrm{ADPc}}{0.64}\right)}\right)^{\mathrm{PK\_n}}\right) \cdot \left(1 + \frac{\mathrm{ADPc}}{\mathrm{KADP\_v12}}\right)} \tag{5}$$

6.6 Function definition function_16

Name Rate Law for glycerol3phosphatedehydrogenase

Arguments Vmax_v8, DHAPg, KDHAPg_v8, NADH, KNADH_v8, r_v8, NAD, KNAD_v8, Gly3Pg, KGly3Pg_v8

Mathematical Expression

$$\mathrm{Vmax\_v8} \cdot \frac{\frac{\mathrm{DHAPg}}{\mathrm{KDHAPg\_v8}} \cdot \frac{\mathrm{NADH}}{\mathrm{KNADH\_v8}} - \mathrm{r\_v8} \cdot \frac{\mathrm{NAD}}{\mathrm{KNAD\_v8}} \cdot \frac{\mathrm{Gly3Pg}}{\mathrm{KGly3Pg\_v8}}}{\left(1 + \frac{\mathrm{DHAPg}}{\mathrm{KDHAPg\_v8}} + \frac{\mathrm{Gly3Pg}}{\mathrm{KGly3Pg\_v8}}\right) \cdot \left(1 + \frac{\mathrm{NADH}}{\mathrm{KNADH\_v8}} + \frac{\mathrm{NAD}}{\mathrm{KNAD\_v8}}\right)} \tag{6}$$

6.7 Function definition function_18

Name Rate Law for phosphoglycerate kinase

Arguments Vmax_v11, BPGA13, KBPGA13_v11, ADPg, KADPg_v11, r_v11, PGA3, KPGA3_v11, ATPg, KATPg_v11

Mathematical Expression

$$\mathrm{Vmax\_v11} \cdot \frac{\frac{\mathrm{BPGA13}}{\mathrm{KBPGA13\_v11}} \cdot \frac{\mathrm{ADPg}}{\mathrm{KADPg\_v11}} - \mathrm{r\_v11} \cdot \frac{\mathrm{PGA3}}{\mathrm{KPGA3\_v11}} \cdot \frac{\mathrm{ATPg}}{\mathrm{KATPg\_v11}}}{\left(1 + \frac{\mathrm{BPGA13}}{\mathrm{KBPGA13\_v11}} + \frac{\mathrm{PGA3}}{\mathrm{KPGA3\_v11}}\right) \cdot \left(1 + \frac{\mathrm{ADPg}}{\mathrm{KADPg\_v11}} + \frac{\mathrm{ATPg}}{\mathrm{KATPg\_v11}}\right)} \tag{7}$$

6.8 Function definition function_13

Name Rate Law for phophofructokinase

Arguments Vmax_v4, Ki1Fru16BP_v4, Fru16BP, Fru6P, KFru6P_v4, ATPg, KATPg_v4, Ki2Fru16BP_v4

Mathematical Expression

$$\frac{\mathrm{Vmax\_v4} \cdot \frac{\mathrm{Ki1Fru16BP\_v4}}{\mathrm{Ki1Fru16BP\_v4} + \mathrm{Fru16BP}} \cdot \frac{\mathrm{Fru6P}}{\mathrm{KFru6P\_v4}} \cdot \frac{\mathrm{ATPg}}{\mathrm{KATPg\_v4}}}{\left(1 + \frac{\mathrm{Fru6P}}{\mathrm{KFru6P\_v4}} + \frac{\mathrm{Fru16BP}}{\mathrm{Ki2Fru16BP\_v4}}\right) \cdot \left(1 + \frac{\mathrm{ATPg}}{\mathrm{KATPg\_v4}}\right)} \tag{8}$$

6.9 Function definition function_21

Name Rate Law for glycerol kinase

Arguments Vmax_v14, Gly3Pg, KGly3Pg_v14, ADPg, KADPg_v14, r_v14, Glycerol, KGlycerol_v14, ATPg, KATPg_v14

Mathematical Expression

$$\mathrm{Vmax\_v14} \cdot \frac{\frac{\mathrm{Gly3Pg}}{\mathrm{KGly3Pg\_v14}} \cdot \frac{\mathrm{ADPg}}{\mathrm{KADPg\_v14}} - \mathrm{r\_v14} \cdot \frac{\mathrm{Glycerol}}{\mathrm{KGlycerol\_v14}} \cdot \frac{\mathrm{ATPg}}{\mathrm{KATPg\_v14}}}{\left(1 + \frac{\mathrm{Gly3Pg}}{\mathrm{KGly3Pg\_v14}} + \frac{\mathrm{Glycerol}}{\mathrm{KGlycerol\_v14}}\right) \cdot \left(1 + \frac{\mathrm{ADPg}}{\mathrm{KADPg\_v14}} + \frac{\mathrm{ATPg}}{\mathrm{KATPg\_v14}}\right)} \tag{9}$$

6.10 Function definition function_11

Name Rate Law for hexokinase

Arguments Vmax_v2, GlucoseInt, KGlcInt_v2, ATPg, KATPg_v2, ADPg, KADPg_v2, Glc6P, KGlc6P_v2

Mathematical Expression

$$\frac{\mathrm{Vmax\_v2} \cdot \frac{\mathrm{GlucoseInt}}{\mathrm{KGlcInt\_v2}} \cdot \frac{\mathrm{ATPg}}{\mathrm{KATPg\_v2}}}{\left(1 + \frac{\mathrm{ATPg}}{\mathrm{KATPg\_v2}} + \frac{\mathrm{ADPg}}{\mathrm{KADPg\_v2}}\right) \cdot \left(1 + \frac{\mathrm{GlucoseInt}}{\mathrm{KGlcInt\_v2}} + \frac{\mathrm{Glc6P}}{\mathrm{KGlc6P\_v2}}\right)} \tag{10}$$

6.11 Function definition function_14

Name Rate Law for aldolase

Arguments Vmax_v5, Fru16BP, GAP, DHAPg, Keq_v5, ATPg, ADPg, AMPg, r_v5, KGAP_v5, KGAPi_v5

Mathematical Expression

$$\frac{\mathrm{Vmax\_v5} \cdot \left(\mathrm{Fru16BP} - \frac{\mathrm{GAP} \cdot \mathrm{DHAPg}}{\mathrm{Keq\_v5}}\right)}{0.0090 \cdot \left(1 + \frac{\mathrm{ATPg}}{0.68} + \frac{\mathrm{ADPg}}{1.51} + \frac{\mathrm{AMPg}}{3.65}\right) + \mathrm{Fru16BP} + \mathrm{GAP} \cdot \frac{0.015 \cdot \left(1 + \frac{\mathrm{ATPg}}{0.68} + \frac{\mathrm{ADPg}}{1.51} + \frac{\mathrm{AMPg}}{3.65}\right)}{\mathrm{Keq\_v5}} \cdot \frac{1}{\mathrm{r\_v5}} + \mathrm{DHAPg} \cdot \frac{\mathrm{KGAP\_v5}}{\mathrm{Keq\_v5}} \cdot \frac{1}{\mathrm{r\_v5}}} \tag{11}$$

6.12 Function definition function_22

Name Rate Law for adenylate kinase

Arguments k, atp, amp, keqak, adp

Mathematical Expression

$$\mathrm{k} \cdot (\mathrm{atp} \cdot \mathrm{amp} - \mathrm{keqak} \cdot \mathrm{adp} \cdot \mathrm{adp}) \tag{12}$$

6.13 Function definition function_10

Name Rate Law for glucose transport

Arguments Vmax_v1, GlucoseExt, GlucoseInt, KGlc, Alpha_v1

Mathematical Expression

$$\mathrm{Vmax\_v1} \cdot \frac{\mathrm{GlucoseExt} - \mathrm{GlucoseInt}}{\mathrm{KGlc} + \mathrm{GlucoseExt} + \mathrm{GlucoseInt} + \frac{\mathrm{Alpha\_v1} \cdot \mathrm{GlucoseExt} \cdot \mathrm{GlucoseInt}}{\mathrm{KGlc}}} \tag{13}$$

7 Reactions

This model contains 21 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

№	Id	Name	Reaction Equation	SBO
1	vGT	glucose transport	$\text{species\_25} \rightleftharpoons \text{species\_10}$	
2	vHK	hexokinase	$\text{species\_10} + \text{species\_11} \rightleftharpoons \text{species\_14} + \text{species\_12}$	
3	vPGI	phosphoglycerate isomerase	$\text{species\_14} \rightleftharpoons \text{species\_15}$	
4	vPFK	phophofructokinase	$\text{species\_15} + \text{species\_11} \rightleftharpoons \text{species\_16} + \text{species\_12}$	
5	vALD	aldolase	$\text{species\_16} \xrightleftharpoons{\text{species\_11, species\_12, species\_13}} \text{species\_17} + \text{species\_18}$	
6	vTPI	triosephosphate isomerase	$\text{species\_17} \rightleftharpoons \text{species\_18}$	
7	vGAPDH	glyceraldehyde3phosphatedehydrogenase	$\text{species\_18} + \text{species\_19} \rightleftharpoons \text{species\_21} + \text{species\_20}$	
8	vGPDH	glycerol3phosphatedehydrogenase	$\text{species\_17} + \text{species\_20} \rightleftharpoons \text{species\_19} + \text{species\_22}$	
9	vGPO	glycerol3phosphate oxidase	$\text{species\_9} \longrightarrow \text{species\_8}$	
10	vPT	pyruvate transport	$\text{species\_1} \longrightarrow \text{species\_26}$	
11	vPGK	phosphoglycerate kinase	$\text{species\_21} + \text{species\_12} \rightleftharpoons \text{species\_23} + \text{species\_11}$	
12	vPK	pyruvate kinase	$\text{species\_4} + \text{species\_2} \rightleftharpoons \text{species\_1} + \text{species\_3}$	
13	vAU	atp utilisation	$\text{species\_3} \longrightarrow \text{species\_2}$	
14	vGK	glycerol kinase	$\text{species\_22} + \text{species\_12} \rightleftharpoons \text{species\_24} + \text{species\_11}$	
15	vPGM	phosphoglycerate mutase	$\text{species\_7} \rightleftharpoons \text{species\_5}$	

№	Id	Name	Reaction Equation	SBO
16	`vENO`	enolase	species_5 $\rightleftharpoons$ species_4	
17	`vAKc`	adenylate kinase cytosol	species_3 + species_6 $\rightleftharpoons$ 2 species_2	
18	`vAKg`	adenylate kinase glycosome	species_11 + species_13 $\rightleftharpoons$ 2 species_12	
19	`vPGT`	3phosphoglycerate transport	species_23 $\rightleftharpoons$ species_7	
20	`vANTI`	gly3p dhap antiporter	species_22 + species_8 $\rightleftharpoons$ species_9 + species_17	
21	`vGlyT`	glycerol transport	species_24 $\rightleftharpoons$ species_27	

7.1 Reaction vGT

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

Name glucose transport

Reaction equation

$$\text{species\_25} \rightleftharpoons \text{species\_10} \tag{14}$$

Reactant

Table 6: Properties of each reactant.

Id	Name	SBO
species_25	glucose external	

Product

Table 7: Properties of each product.

Id	Name	SBO
species_10	glucose	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \text{function\_10}\left(\text{Vmax\_v1}, [\text{species\_25}], [\text{species\_10}], \text{KGlc}, \text{Alpha\_v1}\right) \tag{15}$$

$$\begin{aligned} &\text{function\_10}\left(\text{Vmax\_v1}, \text{GlucoseExt}, \text{GlucoseInt}, \text{KGlc}, \text{Alpha\_v1}\right) \\ &= \text{Vmax\_v1} \cdot \frac{\text{GlucoseExt} - \text{GlucoseInt}}{\text{KGlc} + \text{GlucoseExt} + \text{GlucoseInt} + \frac{\text{Alpha\_v1} \cdot \text{GlucoseExt} \cdot \text{GlucoseInt}}{\text{KGlc}}} \end{aligned} \tag{16}$$

Table 8: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax_v1			108.90		☑
KGlc			1.00		☑
Alpha_v1			0.75		☑

7.2 Reaction vHK

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

Name hexokinase

Reaction equation

$$\text{species\_10} + \text{species\_11} \rightleftharpoons \text{species\_14} + \text{species\_12} \tag{17}$$

Reactants

Table 9: Properties of each reactant.

Id	Name	SBO
species_10	glucose	
species_11	atpg	

Products

Table 10: Properties of each product.

Id	Name	SBO
species_14	glucose6phosphate	
species_12	adpg	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \text{RaHXK} \cdot \text{vol}(\text{compartment\_2}) \cdot \text{function\_11}(\text{Vmax\_v2}, [\text{species\_10}], \text{KGlcInt\_v2}, [\text{species\_11}], \text{KATPg\_v2}, [\text{species\_12}], \text{KADPg\_v2}, [\text{species\_14}], \text{KGlc6P\_v2}) \tag{18}$$

$$\text{function\_11}(\text{Vmax\_v2}, \text{GlucoseInt}, \text{KGlcInt\_v2}, \text{ATPg}, \text{KATPg\_v2}, \text{ADPg}, \text{KADPg\_v2}, \text{Glc6P}, \text{KGlc6P\_v2}) = \frac{\text{Vmax\_v2} \cdot \frac{\text{GlucoseInt}}{\text{KGlcInt\_v2}} \cdot \frac{\text{ATPg}}{\text{KATPg\_v2}}}{\left(1 + \frac{\text{ATPg}}{\text{KATPg\_v2}} + \frac{\text{ADPg}}{\text{KADPg\_v2}}\right) \cdot \left(1 + \frac{\text{GlucoseInt}}{\text{KGlcInt\_v2}} + \frac{\text{Glc6P}}{\text{KGlc6P\_v2}}\right)} \tag{19}$$

$$\text{function\_11}(\text{Vmax\_v2}, \text{GlucoseInt}, \text{KGlcInt\_v2}, \text{ATPg}, \text{KATPg\_v2}, \text{ADPg}, \text{KADPg\_v2}, \text{Glc6P}, \text{KGlc6P\_v2}) = \frac{\text{Vmax\_v2} \cdot \frac{\text{GlucoseInt}}{\text{KGlcInt\_v2}} \cdot \frac{\text{ATPg}}{\text{KATPg\_v2}}}{\left(1 + \frac{\text{ATPg}}{\text{KATPg\_v2}} + \frac{\text{ADPg}}{\text{KADPg\_v2}}\right) \cdot \left(1 + \frac{\text{GlucoseInt}}{\text{KGlcInt\_v2}} + \frac{\text{Glc6P}}{\text{KGlc6P\_v2}}\right)} \tag{20}$$

Table 11: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax_v2			1929.000		☑
KGlcInt_v2			0.100		☑
KATPg_v2			0.116		☑
KADPg_v2			0.126		☑
KGlc6P_v2			12.000		☑

7.3 Reaction vPGI

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

Name phosphoglycerate isomerase

Reaction equation

$$\text{species\_14} \rightleftharpoons \text{species\_15} \tag{21}$$

Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
species_14	glucose6phosphate	

Product

Table 13: Properties of each product.

Id	Name	SBO
species_15	fructose6phosphate	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \mathrm{vol}\left(\mathrm{compartment\_2}\right) \cdot \mathrm{function\_12}\left([\mathrm{species\_14}], [\mathrm{species\_15}], \mathrm{Kms}, \mathrm{Kmp}, \mathrm{Vf}, \mathrm{Vr}\right) \tag{22}$$

$$\mathrm{function\_12}\left(\mathrm{substrate}, \mathrm{product}, \mathrm{Kms}, \mathrm{Kmp}, \mathrm{Vf}, \mathrm{Vr}\right) = \frac{\frac{\mathrm{Vf}\cdot\mathrm{substrate}}{\mathrm{Kms}} - \frac{\mathrm{Vr}\cdot\mathrm{product}}{\mathrm{Kmp}}}{1 + \frac{\mathrm{substrate}}{\mathrm{Kms}} + \frac{\mathrm{product}}{\mathrm{Kmp}}} \tag{23}$$

$$\text{function\_12}\left(\text{substrate}, \text{product}, \text{Kms}, \text{Kmp}, \text{Vf}, \text{Vr}\right) = \frac{\frac{\text{Vf}\cdot\text{substrate}}{\text{Kms}} - \frac{\text{Vr}\cdot\text{product}}{\text{Kmp}}}{1 + \frac{\text{substrate}}{\text{Kms}} + \frac{\text{product}}{\text{Kmp}}} \tag{24}$$

Table 14: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Kms			0.40		☑
Kmp			0.12		☑
Vf			1305.00		☑
Vr			1305.00		☑

7.4 Reaction vPFK

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

Name phophofructokinase

Reaction equation

$$\text{species\_15} + \text{species\_11} \rightleftharpoons \text{species\_16} + \text{species\_12} \tag{25}$$

Reactants

Table 15: Properties of each reactant.

Id	Name	SBO
species_15	fructose6phosphate	
species_11	atpg	

Products

Table 16: Properties of each product.

Id	Name	SBO
species_16	fructose16bisphosphate	
species_12	adpg	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \mathrm{RaPFK} \cdot \mathrm{vol}\left(\mathrm{compartment\_2}\right) \cdot \mathrm{function\_13}\left(\mathrm{Vmax\_v4}, \mathrm{Ki1Fru16BP\_v4}, \left[\mathrm{species\_16}\right], \left[\mathrm{species\_15}\right], \mathrm{KFru6P\_v4}, \left[\mathrm{species\_11}\right], \mathrm{KATPg\_v4}, \mathrm{Ki2Fru16BP\_v4}\right) \tag{26}$$

$$\mathrm{function\_13}\left(\mathrm{Vmax\_v4}, \mathrm{Ki1Fru16BP\_v4}, \mathrm{Fru16BP}, \mathrm{Fru6P}, \mathrm{KFru6P\_v4}, \mathrm{ATPg}, \mathrm{KATPg\_v4}, \mathrm{Ki2Fru16BP\_v4}\right) = \frac{\mathrm{Vmax\_v4} \cdot \frac{\mathrm{Ki1Fru16BP\_v4}}{\mathrm{Ki1Fru16BP\_v4}+\mathrm{Fru16BP}} \cdot \frac{\mathrm{Fru6P}}{\mathrm{KFru6P\_v4}} \cdot \frac{\mathrm{ATPg}}{\mathrm{KATPg\_v4}}}{\left(1 + \frac{\mathrm{Fru6P}}{\mathrm{KFru6P\_v4}} + \frac{\mathrm{Fru16BP}}{\mathrm{Ki2Fru16BP\_v4}}\right) \cdot \left(1 + \frac{\mathrm{ATPg}}{\mathrm{KATPg\_v4}}\right)} \tag{27}$$

$$\mathrm{function\_13}\left(\mathrm{Vmax\_v4}, \mathrm{Ki1Fru16BP\_v4}, \mathrm{Fru16BP}, \mathrm{Fru6P}, \mathrm{KFru6P\_v4}, \mathrm{ATPg}, \mathrm{KATPg\_v4}, \mathrm{Ki2Fru16BP\_v4}\right) = \frac{\mathrm{Vmax\_v4} \cdot \frac{\mathrm{Ki1Fru16BP\_v4}}{\mathrm{Ki1Fru16BP\_v4}+\mathrm{Fru16BP}} \cdot \frac{\mathrm{Fru6P}}{\mathrm{KFru6P\_v4}} \cdot \frac{\mathrm{ATPg}}{\mathrm{KATPg\_v4}}}{\left(1 + \frac{\mathrm{Fru6P}}{\mathrm{KFru6P\_v4}} + \frac{\mathrm{Fru16BP}}{\mathrm{Ki2Fru16BP\_v4}}\right) \cdot \left(1 + \frac{\mathrm{ATPg}}{\mathrm{KATPg\_v4}}\right)} \tag{28}$$

Table 17: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
`Vmax_v4`			1708.000		☑
`Ki1Fru16BP_v4`			15.800		☑
`KFru6P_v4`			0.820		☑
`KATPg_v4`			0.026		☑
`Ki2Fru16BP_v4`			10.700		☑

7.5 Reaction `vALD`

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

Name aldolase

Reaction equation

$$\mathrm{species\_16} \xrightleftharpoons{\mathrm{species\_11},\ \mathrm{species\_12},\ \mathrm{species\_13}} \mathrm{species\_17} + \mathrm{species\_18} \tag{29}$$

Reactant

Table 18: Properties of each reactant.

Id	Name	SBO
`species_16`	fructose16bisphosphate	

Modifiers

Table 19: Properties of each modifier.

Id	Name	SBO
`species_11`	atpg	
`species_12`	adpg	
`species_13`	ampg	

Products

Table 20: Properties of each product.

Id	Name	SBO
`species_17`	dihydroxyacetonephosphate	
`species_18`	glyceraldehyde3phosphate	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \mathrm{vol}\,(\mathrm{compartment\_2}) \cdot \mathrm{function\_14}\,(\mathrm{Vmax\_v5}, [\mathrm{species\_16}], [\mathrm{species\_18}], [\mathrm{species\_17}], \mathrm{Keq\_v5}, [\mathrm{species\_11}], [\mathrm{species\_12}], [\mathrm{species\_13}], \mathrm{r\_v5}, \mathrm{KGAP\_v5}, \mathrm{KGAPi\_v5}) \quad (30)$$

$$\mathrm{function\_14}\,(\mathrm{Vmax\_v5}, \mathrm{Fru16BP}, \mathrm{GAP}, \mathrm{DHAPg}, \mathrm{Keq\_v5}, \mathrm{ATPg}, \mathrm{ADPg}, \mathrm{AMPg}, \mathrm{r\_v5}, \mathrm{KGAP\_v5}, \mathrm{KGAPi\_v5}) = \frac{\mathrm{Vmax\_v5} \cdot \left(\mathrm{Fru16BP} - \frac{\mathrm{GAP} \cdot \mathrm{DHAPg}}{\mathrm{Keq\_v5}}\right)}{0.0090 \cdot \left(1 + \frac{\mathrm{ATPg}}{0.68} + \frac{\mathrm{ADPg}}{1.51} + \frac{\mathrm{AMPg}}{3.65}\right) + \mathrm{Fru16BP} + \mathrm{GAP} \cdot \frac{0.015 \cdot \left(1 + \frac{\mathrm{ATPg}}{0.68} + \frac{\mathrm{ADPg}}{1.51} + \frac{\mathrm{AMPg}}{3.65}\right)}{\mathrm{Keq\_v5}} \cdot \frac{1}{\mathrm{r\_v5}} + \mathrm{DHAPg} \cdot \frac{\mathrm{KGAP\_v5}}{\mathrm{Keq\_v5}} \cdot \ldots} \quad (31)$$

$$\mathrm{function\_14}\,(\mathrm{Vmax\_v5}, \mathrm{Fru16BP}, \mathrm{GAP}, \mathrm{DHAPg}, \mathrm{Keq\_v5}, \mathrm{ATPg}, \mathrm{ADPg}, \mathrm{AMPg}, \mathrm{r\_v5}, \mathrm{KGAP\_v5}, \mathrm{KGAPi\_v5}) = \frac{\mathrm{Vmax\_v5} \cdot \left(\mathrm{Fru16BP} - \frac{\mathrm{GAP} \cdot \mathrm{DHAPg}}{\mathrm{Keq\_v5}}\right)}{0.0090 \cdot \left(1 + \frac{\mathrm{ATPg}}{0.68} + \frac{\mathrm{ADPg}}{1.51} + \frac{\mathrm{AMPg}}{3.65}\right) + \mathrm{Fru16BP} + \mathrm{GAP} \cdot \frac{0.015 \cdot \left(1 + \frac{\mathrm{ATPg}}{0.68} + \frac{\mathrm{ADPg}}{1.51} + \frac{\mathrm{AMPg}}{3.65}\right)}{\mathrm{Keq\_v5}} \cdot \frac{1}{\mathrm{r\_v5}} + \mathrm{DHAPg} \cdot \frac{\mathrm{KGAP\_v5}}{\mathrm{Keq\_v5}} \cdot \ldots} \quad (32)$$

Table 21: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax_v5			560.000		☑
Keq_v5			0.069		☑
r_v5			1.190		☑
KGAP_v5			0.067		☑
KGAPi_v5			0.098		☑

7.6 Reaction vTPI

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

Name triosephosphate isomerase

Reaction equation

$$\text{species\_17} \rightleftharpoons \text{species\_18} \tag{33}$$

Reactant

Table 22: Properties of each reactant.

Id	Name	SBO
species_17	dihydroxyacetonephosphate	

Product

Table 23: Properties of each product.

Id	Name	SBO
species_18	glyceraldehyde3phosphate	

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \mathrm{vol}\left(\mathrm{compartment\_2}\right) \cdot \mathrm{function\_12}\left([\mathrm{species\_17}], [\mathrm{species\_18}], \mathrm{Kms}, \mathrm{Kmp}, \mathrm{Vf}, \mathrm{Vr}\right) \tag{34}$$

$$\mathrm{function\_12}\left(\mathrm{substrate}, \mathrm{product}, \mathrm{Kms}, \mathrm{Kmp}, \mathrm{Vf}, \mathrm{Vr}\right) = \frac{\frac{\mathrm{Vf} \cdot \mathrm{substrate}}{\mathrm{Kms}} - \frac{\mathrm{Vr} \cdot \mathrm{product}}{\mathrm{Kmp}}}{1 + \frac{\mathrm{substrate}}{\mathrm{Kms}} + \frac{\mathrm{product}}{\mathrm{Kmp}}} \tag{35}$$

$$\mathrm{function\_12}\left(\mathrm{substrate}, \mathrm{product}, \mathrm{Kms}, \mathrm{Kmp}, \mathrm{Vf}, \mathrm{Vr}\right) = \frac{\frac{\mathrm{Vf} \cdot \mathrm{substrate}}{\mathrm{Kms}} - \frac{\mathrm{Vr} \cdot \mathrm{product}}{\mathrm{Kmp}}}{1 + \frac{\mathrm{substrate}}{\mathrm{Kms}} + \frac{\mathrm{product}}{\mathrm{Kmp}}} \quad (36)$$

Table 24: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Kms			1.20		☑
Kmp			0.25		☑
Vf			999.30		☑
Vr			5696.01		☑

7.7 Reaction vGAPDH

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

Name glyceraldehyde3phosphatedehydrogenase

Reaction equation

$$\mathrm{species\_18} + \mathrm{species\_19} \rightleftharpoons \mathrm{species\_21} + \mathrm{species\_20} \quad (37)$$

Reactants

Table 25: Properties of each reactant.

Id	Name	SBO
species_18	glyceraldehyde3phosphate	
species_19	nad	

Products

Table 26: Properties of each product.

Id	Name	SBO
species_21	bisphosphoglycerate	
species_20	nadh	

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \mathrm{vol}\left(\mathrm{compartment\_2}\right) \cdot \mathrm{function\_15}\left(\mathrm{Vmax\_v7}, [\mathrm{species\_18}], \mathrm{KGAP\_v7}, [\mathrm{species\_19}], \mathrm{KNAD\_v7}, \mathrm{r\_v7}, [\mathrm{species\_21}], \mathrm{KBPGA13\_v7}, [\mathrm{species\_20}], \mathrm{KNADH\_v7}\right) \quad (38)$$

$$\mathrm{function\_15}\left(\mathrm{Vmax\_v7}, \mathrm{GAP}, \mathrm{KGAP\_v7}, \mathrm{NAD}, \mathrm{KNAD\_v7}, \mathrm{r\_v7}, \mathrm{BPGA13}, \mathrm{KBPGA13\_v7}, \mathrm{NADH}, \mathrm{KNADH\_v7}\right) = \mathrm{Vmax\_v7} \cdot \frac{\frac{\mathrm{GAP}}{\mathrm{KGAP\_v7}} \cdot \frac{\mathrm{NAD}}{\mathrm{KNAD\_v7}} - \mathrm{r\_v7} \cdot \frac{\mathrm{BPGA13}}{\mathrm{KBPGA13\_v7}} \cdot \frac{\mathrm{NADH}}{\mathrm{KNADH\_v7}}}{\left(1 + \frac{\mathrm{GAP}}{\mathrm{KGAP\_v7}} + \frac{\mathrm{BPGA13}}{\mathrm{KBPGA13\_v7}}\right) \cdot \left(1 + \frac{\mathrm{NAD}}{\mathrm{KNAD\_v7}} + \frac{\mathrm{NADH}}{\mathrm{KNADH\_v7}}\right)} \quad (39)$$

$$\mathrm{function\_15}\left(\mathrm{Vmax\_v7}, \mathrm{GAP}, \mathrm{KGAP\_v7}, \mathrm{NAD}, \mathrm{KNAD\_v7}, \mathrm{r\_v7}, \mathrm{BPGA13}, \mathrm{KBPGA13\_v7}, \mathrm{NADH}, \mathrm{KNADH\_v7}\right) = \mathrm{Vmax\_v7} \cdot \frac{\frac{\mathrm{GAP}}{\mathrm{KGAP\_v7}} \cdot \frac{\mathrm{NAD}}{\mathrm{KNAD\_v7}} - \mathrm{r\_v7} \cdot \frac{\mathrm{BPGA13}}{\mathrm{KBPGA13\_v7}} \cdot \frac{\mathrm{NADH}}{\mathrm{KNADH\_v7}}}{\left(1 + \frac{\mathrm{GAP}}{\mathrm{KGAP\_v7}} + \frac{\mathrm{BPGA13}}{\mathrm{KBPGA13\_v7}}\right) \cdot \left(1 + \frac{\mathrm{NAD}}{\mathrm{KNAD\_v7}} + \frac{\mathrm{NADH}}{\mathrm{KNADH\_v7}}\right)} \quad (40)$$

Table 27: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax_v7			720.90		☑
KGAP_v7			0.15		☑
KNAD_v7			0.45		☑
r_v7			0.67		☑
KBPGA13_v7			0.10		☑
KNADH_v7			0.02		☑

7.8 Reaction vGPDH

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

Name glycerol3phosphatedehydrogenase

Reaction equation

$$\mathrm{species\_17} + \mathrm{species\_20} \rightleftharpoons \mathrm{species\_19} + \mathrm{species\_22} \quad (41)$$

Reactants

Table 28: Properties of each reactant.

Id	Name	SBO
species_17	dihydroxyacetonephosphate	

Id	Name	SBO
species_20	nadh	

Products

Table 29: Properties of each product.

Id	Name	SBO
species_19	nad	
species_22	glycerol3phosphate	

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \mathrm{vol}\left(\mathrm{compartment\_2}\right) \cdot \mathrm{function\_16}\left(\mathrm{Vmax\_v8}, [\mathrm{species\_17}], \mathrm{KDHAPg\_v8}, [\mathrm{species\_20}], \mathrm{KNADH\_v8}, \mathrm{r\_v8}, [\mathrm{species\_19}], \mathrm{KNAD\_v8}, [\mathrm{species\_22}], \mathrm{KGly3Pg\_v8}\right) \tag{42}$$

$$\mathrm{function\_16}\left(\mathrm{Vmax\_v8}, \mathrm{DHAPg}, \mathrm{KDHAPg\_v8}, \mathrm{NADH}, \mathrm{KNADH\_v8}, \mathrm{r\_v8}, \mathrm{NAD}, \mathrm{KNAD\_v8}, \mathrm{Gly3Pg}, \mathrm{KGly3Pg\_v8}\right) = \mathrm{Vmax\_v8} \cdot \frac{\frac{\mathrm{DHAPg}}{\mathrm{KDHAPg\_v8}} \cdot \frac{\mathrm{NADH}}{\mathrm{KNADH\_v8}} - \mathrm{r\_v8} \cdot \frac{\mathrm{NAD}}{\mathrm{KNAD\_v8}} \cdot \frac{\mathrm{Gly3Pg}}{\mathrm{KGly3Pg\_v8}}}{\left(1 + \frac{\mathrm{DHAPg}}{\mathrm{KDHAPg\_v8}} + \frac{\mathrm{Gly3Pg}}{\mathrm{KGly3Pg\_v8}}\right) \cdot \left(1 + \frac{\mathrm{NADH}}{\mathrm{KNADH\_v8}} + \frac{\mathrm{NAD}}{\mathrm{KNAD\_v8}}\right)} \tag{43}$$

$$\mathrm{function\_16}\left(\mathrm{Vmax\_v8}, \mathrm{DHAPg}, \mathrm{KDHAPg\_v8}, \mathrm{NADH}, \mathrm{KNADH\_v8}, \mathrm{r\_v8}, \mathrm{NAD}, \mathrm{KNAD\_v8}, \mathrm{Gly3Pg}, \mathrm{KGly3Pg\_v8}\right) = \mathrm{Vmax\_v8} \cdot \frac{\frac{\mathrm{DHAPg}}{\mathrm{KDHAPg\_v8}} \cdot \frac{\mathrm{NADH}}{\mathrm{KNADH\_v8}} - \mathrm{r\_v8} \cdot \frac{\mathrm{NAD}}{\mathrm{KNAD\_v8}} \cdot \frac{\mathrm{Gly3Pg}}{\mathrm{KGly3Pg\_v8}}}{\left(1 + \frac{\mathrm{DHAPg}}{\mathrm{KDHAPg\_v8}} + \frac{\mathrm{Gly3Pg}}{\mathrm{KGly3Pg\_v8}}\right) \cdot \left(1 + \frac{\mathrm{NADH}}{\mathrm{KNADH\_v8}} + \frac{\mathrm{NAD}}{\mathrm{KNAD\_v8}}\right)} \tag{44}$$

Table 30: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax_v8			465.00		☑
KDHAPg_v8			0.10		☑
KNADH_v8			0.01		☑
r_v8			0.28		☑
KNAD_v8			0.40		☑
KGly3Pg_v8			2.00		☑

7.9 Reaction vGPO

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

Name glycerol3phosphate oxidase

Reaction equation

$$\text{species\_9} \longrightarrow \text{species\_8} \tag{45}$$

Reactant

Table 31: Properties of each reactant.

Id	Name	SBO
species_9	glycerol3phosphate cytosol	

Product

Table 32: Properties of each product.

Id	Name	SBO
species_8	dihydroxyacetonephosphate cytosol	

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \mathrm{vol}\left(\text{compartment\_1}\right) \cdot \text{function\_17}\left(\left[\text{species\_9}\right], \text{Km}, \text{V}\right) \tag{46}$$

$$\text{function\_17}\left(\text{substrate}, \text{Km}, \text{V}\right) = \frac{\text{V} \cdot \text{substrate}}{\text{Km} + \text{substrate}} \tag{47}$$

$$\text{function\_17}\left(\text{substrate}, \text{Km}, \text{V}\right) = \frac{\text{V} \cdot \text{substrate}}{\text{Km} + \text{substrate}} \tag{48}$$

Table 33: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Km			1.7		☑
V			368.0		☑

7.10 Reaction vPT

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

Name pyruvate transport

Reaction equation

$$\text{species\_1} \longrightarrow \text{species\_26} \tag{49}$$

Reactant

Table 34: Properties of each reactant.

Id	Name	SBO
species_1	pyruvate	

Product

Table 35: Properties of each product.

Id	Name	SBO
species_26	pyruvate external	

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = \text{function\_17}\left([\text{species\_1}], \text{Km}, \text{V}\right) \tag{50}$$

$$\text{function\_17}\left(\text{substrate}, \text{Km}, \text{V}\right) = \frac{\text{V} \cdot \text{substrate}}{\text{Km} + \text{substrate}} \tag{51}$$

Table 36: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Km			1.96		☑
V			200.00		☑

7.11 Reaction vPGK

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

Name phosphoglycerate kinase

Reaction equation

$$\text{species\_21} + \text{species\_12} \rightleftharpoons \text{species\_23} + \text{species\_11} \tag{52}$$

Reactants

Table 37: Properties of each reactant.

Id	Name	SBO
species_21	bisphosphoglycerate	
species_12	adpg	

Products

Table 38: Properties of each product.

Id	Name	SBO
species_23	3phosphoglycerate	
species_11	atpg	

Kinetic Law

Derived unit contains undeclared units

$$\begin{aligned} v_{11} = &\ \mathrm{vol}(\text{compartment\_2}) \cdot \text{function\_18}(\text{Vmax\_v11}, [\text{species\_21}], \text{KBPGA13\_v11}, \\ &[\text{species\_12}], \text{KADPg\_v11}, \text{r\_v11}, [\text{species\_23}], \text{KPGA3\_v11}, [\text{species\_11}], \text{KATPg\_v11}) \end{aligned} \tag{53}$$

$$\begin{aligned} &\text{function\_18}(\text{Vmax\_v11}, \text{BPGA13}, \text{KBPGA13\_v11}, \text{ADPg}, \text{KADPg\_v11}, \\ &\text{r\_v11}, \text{PGA3}, \text{KPGA3\_v11}, \text{ATPg}, \text{KATPg\_v11}) = \text{Vmax\_v11} \\ &\cdot \frac{\frac{\text{BPGA13}}{\text{KBPGA13\_v11}} \cdot \frac{\text{ADPg}}{\text{KADPg\_v11}} - \text{r\_v11} \cdot \frac{\text{PGA3}}{\text{KPGA3\_v11}} \cdot \frac{\text{ATPg}}{\text{KATPg\_v11}}}{\left(1 + \frac{\text{BPGA13}}{\text{KBPGA13\_v11}} + \frac{\text{PGA3}}{\text{KPGA3\_v11}}\right) \cdot \left(1 + \frac{\text{ADPg}}{\text{KADPg\_v11}} + \frac{\text{ATPg}}{\text{KATPg\_v11}}\right)} \end{aligned} \tag{54}$$

$$\begin{aligned} &\text{function\_18}\,(\text{Vmax\_v11}, \text{BPGA13}, \text{KBPGA13\_v11}, \text{ADPg}, \text{KADPg\_v11},\\ &\text{r\_v11}, \text{PGA3}, \text{KPGA3\_v11}, \text{ATPg}, \text{KATPg\_v11}) = \text{Vmax\_v11}\\ &\cdot \frac{\frac{\text{BPGA13}}{\text{KBPGA13\_v11}} \cdot \frac{\text{ADPg}}{\text{KADPg\_v11}} - \text{r\_v11} \cdot \frac{\text{PGA3}}{\text{KPGA3\_v11}} \cdot \frac{\text{ATPg}}{\text{KATPg\_v11}}}{\left(1 + \frac{\text{BPGA13}}{\text{KBPGA13\_v11}} + \frac{\text{PGA3}}{\text{KPGA3\_v11}}\right) \cdot \left(1 + \frac{\text{ADPg}}{\text{KADPg\_v11}} + \frac{\text{ATPg}}{\text{KATPg\_v11}}\right)} \end{aligned} \tag{55}$$

Table 39: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax_v11			2862.000		☑
KBPGA13_v11			0.003		☑
KADPg_v11			0.100		☑
r_v11			0.470		☑
KPGA3_v11			1.620		☑
KATPg_v11			0.290		☑

7.12 Reaction vPK

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

Name pyruvate kinase

Reaction equation

$$\text{species\_4} + \text{species\_2} \rightleftharpoons \text{species\_1} + \text{species\_3} \tag{56}$$

Reactants

Table 40: Properties of each reactant.

Id	Name	SBO
species_4	phosphoenolpyruvate	
species_2	adpc	

Products

Table 41: Properties of each product.

Id	Name	SBO
species_1	pyruvate	
species_3	atpc	

Id	Name	SBO

Kinetic Law

Derived unit contains undeclared units

$$v_{12} = \mathrm{RaPYK} \cdot \mathrm{vol}\left(\mathrm{compartment\_1}\right) \cdot \mathrm{function\_19}\left(\mathrm{Vmax\_v12}, [\mathrm{species\_4}], \mathrm{PK\_n}, [\mathrm{species\_2}], \mathrm{KADP\_v12}, [\mathrm{species\_3}]\right) \tag{57}$$

$$\mathrm{function\_19}\left(\mathrm{Vmax\_v12}, \mathrm{PEP}, \mathrm{PK\_n}, \mathrm{ADPc}, \mathrm{KADP\_v12}, \mathrm{ATPc}\right) = \frac{\mathrm{Vmax\_v12} \cdot \left(\frac{\mathrm{PEP}}{0.34 \cdot \left(1 + \frac{\mathrm{ATPc}}{0.57} + \frac{\mathrm{ADPc}}{0.64}\right)}\right)^{\mathrm{PK\_n}} \cdot \frac{\mathrm{ADPc}}{\mathrm{KADP\_v12}}}{\left(1 + \left(\frac{\mathrm{PEP}}{0.34 \cdot \left(1 + \frac{\mathrm{ATPc}}{0.57} + \frac{\mathrm{ADPc}}{0.64}\right)}\right)^{\mathrm{PK\_n}}\right) \cdot \left(1 + \frac{\mathrm{ADPc}}{\mathrm{KADP\_v12}}\right)} \tag{58}$$

$$\mathrm{function\_19}\left(\mathrm{Vmax\_v12}, \mathrm{PEP}, \mathrm{PK\_n}, \mathrm{ADPc}, \mathrm{KADP\_v12}, \mathrm{ATPc}\right) = \frac{\mathrm{Vmax\_v12} \cdot \left(\frac{\mathrm{PEP}}{0.34 \cdot \left(1 + \frac{\mathrm{ATPc}}{0.57} + \frac{\mathrm{ADPc}}{0.64}\right)}\right)^{\mathrm{PK\_n}} \cdot \frac{\mathrm{ADPc}}{\mathrm{KADP\_v12}}}{\left(1 + \left(\frac{\mathrm{PEP}}{0.34 \cdot \left(1 + \frac{\mathrm{ATPc}}{0.57} + \frac{\mathrm{ADPc}}{0.64}\right)}\right)^{\mathrm{PK\_n}}\right) \cdot \left(1 + \frac{\mathrm{ADPc}}{\mathrm{KADP\_v12}}\right)} \tag{59}$$

Table 42: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax_v12			1020.000		☑
PK_n			2.500		☑
KADP_v12			0.114		☑

7.13 Reaction vAU

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

Name atp utilisation

Reaction equation

$$\mathrm{species\_3} \longrightarrow \mathrm{species\_2} \tag{60}$$

Reactant

Table 43: Properties of each reactant.

Id	Name	SBO
species_3	atpc	

Product

Table 44: Properties of each product.

Id	Name	SBO
species_2	adpc	

Kinetic Law

Derived unit contains undeclared units

$$v_{13} = \mathrm{vol}\left(\mathrm{compartment\_1}\right) \cdot \mathrm{function\_20}\left(\mathrm{k}, [\mathrm{species\_3}], [\mathrm{species\_2}]\right) \tag{61}$$

$$\mathrm{function\_20}\left(\mathrm{k}, \mathrm{atpc}, \mathrm{adpc}\right) = \frac{\mathrm{k} \cdot \mathrm{atpc}}{\mathrm{adpc}} \tag{62}$$

$$\mathrm{function\_20}\left(\mathrm{k}, \mathrm{atpc}, \mathrm{adpc}\right) = \frac{\mathrm{k} \cdot \mathrm{atpc}}{\mathrm{adpc}} \tag{63}$$

Table 45: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k			50.0		☑

7.14 Reaction vGK

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

Name glycerol kinase

Reaction equation

$$\mathrm{species\_22} + \mathrm{species\_12} \rightleftharpoons \mathrm{species\_24} + \mathrm{species\_11} \tag{64}$$

Reactants

Table 46: Properties of each reactant.

Id	Name	SBO
species_22	glycerol3phosphate	
species_12	adpg	

Products

Table 47: Properties of each product.

Id	Name	SBO
species_24	glycerol	
species_11	atpg	

Kinetic Law

Derived unit contains undeclared units

$$v_{14} = \mathrm{vol}\left(\mathrm{compartment\_2}\right) \cdot \mathrm{function\_21}\left(\mathrm{Vmax\_v14}, [\mathrm{species\_22}], \mathrm{KGly3Pg\_v14}, [\mathrm{species\_12}], \mathrm{KADPg\_v14}, \mathrm{r\_v14}, [\mathrm{species\_24}], \mathrm{KGlycerol\_v14}, [\mathrm{species\_11}], \mathrm{KATPg\_v14}\right) \tag{65}$$

$$\mathrm{function\_21}\left(\mathrm{Vmax\_v14}, \mathrm{Gly3Pg}, \mathrm{KGly3Pg\_v14}, \mathrm{ADPg}, \mathrm{KADPg\_v14}, \mathrm{r\_v14}, \mathrm{Glycerol}, \mathrm{KGlycerol\_v14}, \mathrm{ATPg}, \mathrm{KATPg\_v14}\right) = \mathrm{Vmax\_v14} \cdot \frac{\frac{\mathrm{Gly3Pg}}{\mathrm{KGly3Pg\_v14}} \cdot \frac{\mathrm{ADPg}}{\mathrm{KADPg\_v14}} - \mathrm{r\_v14} \cdot \frac{\mathrm{Glycerol}}{\mathrm{KGlycerol\_v14}} \cdot \frac{\mathrm{ATPg}}{\mathrm{KATPg\_v14}}}{\left(1 + \frac{\mathrm{Gly3Pg}}{\mathrm{KGly3Pg\_v14}} + \frac{\mathrm{Glycerol}}{\mathrm{KGlycerol\_v14}}\right) \cdot \left(1 + \frac{\mathrm{ADPg}}{\mathrm{KADPg\_v14}} + \frac{\mathrm{ATPg}}{\mathrm{KATPg\_v14}}\right)} \tag{66}$$

$$\mathrm{function\_21}\left(\mathrm{Vmax\_v14}, \mathrm{Gly3Pg}, \mathrm{KGly3Pg\_v14}, \mathrm{ADPg}, \mathrm{KADPg\_v14}, \mathrm{r\_v14}, \mathrm{Glycerol}, \mathrm{KGlycerol\_v14}, \mathrm{ATPg}, \mathrm{KATPg\_v14}\right) = \mathrm{Vmax\_v14} \cdot \frac{\frac{\mathrm{Gly3Pg}}{\mathrm{KGly3Pg\_v14}} \cdot \frac{\mathrm{ADPg}}{\mathrm{KADPg\_v14}} - \mathrm{r\_v14} \cdot \frac{\mathrm{Glycerol}}{\mathrm{KGlycerol\_v14}} \cdot \frac{\mathrm{ATPg}}{\mathrm{KATPg\_v14}}}{\left(1 + \frac{\mathrm{Gly3Pg}}{\mathrm{KGly3Pg\_v14}} + \frac{\mathrm{Glycerol}}{\mathrm{KGlycerol\_v14}}\right) \cdot \left(1 + \frac{\mathrm{ADPg}}{\mathrm{KADPg\_v14}} + \frac{\mathrm{ATPg}}{\mathrm{KATPg\_v14}}\right)} \tag{67}$$

Table 48: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax_v14			200.00		☑

Id	Name	SBO	Value	Unit	Constant
KGly3Pg_v14			3.83		☑
KADPg_v14			0.56		☑
r_v14			60.86		☑
KGlycerol-_v14			0.44		☑
KATPg_v14			0.24		☑

7.15 Reaction vPGM

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

Name phosphoglycerate mutase

Reaction equation

$$\text{species\_7} \rightleftharpoons \text{species\_5} \tag{68}$$

Reactant

Table 49: Properties of each reactant.

Id	Name	SBO
species_7	3phosphoglycerate cytosol	

Product

Table 50: Properties of each product.

Id	Name	SBO
species_5	2phosphoglycerate	

Kinetic Law

Derived unit contains undeclared units

$$v_{15} = \text{RaPGAM} \cdot \text{vol}\left(\text{compartment\_1}\right) \cdot \text{function\_12}\left([\text{species\_7}], [\text{species\_5}], \text{Kms}, \text{Kmp}, \text{Vf}, \text{Vr}\right) \tag{69}$$

$$\text{function\_12}\left(\text{substrate}, \text{product}, \text{Kms}, \text{Kmp}, \text{Vf}, \text{Vr}\right) = \frac{\frac{\text{Vf}\cdot\text{substrate}}{\text{Kms}} - \frac{\text{Vr}\cdot\text{product}}{\text{Kmp}}}{1 + \frac{\text{substrate}}{\text{Kms}} + \frac{\text{product}}{\text{Kmp}}} \tag{70}$$

$$\text{function\_12}\left(\text{substrate}, \text{product}, \text{Kms}, \text{Kmp}, \text{Vf}, \text{Vr}\right) = \frac{\frac{\text{Vf} \cdot \text{substrate}}{\text{Kms}} - \frac{\text{Vr} \cdot \text{product}}{\text{Kmp}}}{1 + \frac{\text{substrate}}{\text{Kms}} + \frac{\text{product}}{\text{Kmp}}} \tag{71}$$

Table 51: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Kms			0.27		☑
Kmp			0.11		☑
Vf			225.00		☑
Vr			495.00		☑

7.16 Reaction vENO

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

Name enolase

Reaction equation

$$\text{species\_5} \rightleftharpoons \text{species\_4} \tag{72}$$

Reactant

Table 52: Properties of each reactant.

Id	Name	SBO
species_5	2phosphoglycerate	

Product

Table 53: Properties of each product.

Id	Name	SBO
species_4	phosphoenolpyruvate	

Kinetic Law

Derived unit contains undeclared units

$$v_{16} = \text{RaENO} \cdot \text{vol}\left(\text{compartment\_1}\right) \cdot \text{function\_12}\left(\left[\text{species\_5}\right], \left[\text{species\_4}\right], \text{Kms}, \text{Kmp}, \text{Vf}, \text{Vr}\right) \tag{73}$$

$$\text{function\_12}\left(\text{substrate}, \text{product}, \text{Kms}, \text{Kmp}, \text{Vf}, \text{Vr}\right) = \frac{\frac{\text{Vf}\cdot\text{substrate}}{\text{Kms}} - \frac{\text{Vr}\cdot\text{product}}{\text{Kmp}}}{1 + \frac{\text{substrate}}{\text{Kms}} + \frac{\text{product}}{\text{Kmp}}} \quad (74)$$

$$\text{function\_12}\left(\text{substrate}, \text{product}, \text{Kms}, \text{Kmp}, \text{Vf}, \text{Vr}\right) = \frac{\frac{\text{Vf}\cdot\text{substrate}}{\text{Kms}} - \frac{\text{Vr}\cdot\text{product}}{\text{Kmp}}}{1 + \frac{\text{substrate}}{\text{Kms}} + \frac{\text{product}}{\text{Kmp}}} \quad (75)$$

Table 54: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Kms			0.054		☑
Kmp			0.240		☑
Vf			598.000		☑
Vr			394.680		☑

7.17 Reaction vAKc

This is a reversible reaction of two reactants forming one product.

Name adenylate kinase cytosol

Reaction equation

$$\text{species\_3} + \text{species\_6} \rightleftharpoons 2\,\text{species\_2} \quad (76)$$

Reactants

Table 55: Properties of each reactant.

Id	Name	SBO
species_3	atpc	
species_6	ampc	

Product

Table 56: Properties of each product.

Id	Name	SBO
species_2	adpc	

Kinetic Law

Derived unit contains undeclared units

$$v_{17} = \mathrm{vol}\,(\mathrm{compartment\_1}) \cdot \mathrm{function\_22}\,(\mathrm{k}, [\mathrm{species\_3}], [\mathrm{species\_6}], \mathrm{keqak}, [\mathrm{species\_2}]) \tag{77}$$

$$\mathrm{function\_22}\,(\mathrm{k}, \mathrm{atp}, \mathrm{amp}, \mathrm{keqak}, \mathrm{adp}) = \mathrm{k} \cdot (\mathrm{atp} \cdot \mathrm{amp} - \mathrm{keqak} \cdot \mathrm{adp} \cdot \mathrm{adp}) \tag{78}$$

$$\mathrm{function\_22}\,(\mathrm{k}, \mathrm{atp}, \mathrm{amp}, \mathrm{keqak}, \mathrm{adp}) = \mathrm{k} \cdot (\mathrm{atp} \cdot \mathrm{amp} - \mathrm{keqak} \cdot \mathrm{adp} \cdot \mathrm{adp}) \tag{79}$$

Table 57: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k			1000000.000		☑
keqak			0.442		☑

7.18 Reaction vAKg

This is a reversible reaction of two reactants forming one product.

Name adenylate kinase glycosome

Reaction equation

$$\mathrm{species\_11} + \mathrm{species\_13} \rightleftharpoons 2\,\mathrm{species\_12} \tag{80}$$

Reactants

Table 58: Properties of each reactant.

Id	Name	SBO
species_11	atpg	
species_13	ampg	

Product

Table 59: Properties of each product.

Id	Name	SBO
species_12	adpg	

Kinetic Law

Derived unit contains undeclared units

$$v_{18} = \mathrm{vol}\left(\mathrm{compartment\_2}\right) \cdot \mathrm{function\_22}\left(\mathrm{k}, [\mathrm{species\_11}], [\mathrm{species\_13}], \mathrm{keqak}, [\mathrm{species\_12}]\right) \quad (81)$$

$$\mathrm{function\_22}\left(\mathrm{k}, \mathrm{atp}, \mathrm{amp}, \mathrm{keqak}, \mathrm{adp}\right) = \mathrm{k} \cdot \left(\mathrm{atp} \cdot \mathrm{amp} - \mathrm{keqak} \cdot \mathrm{adp} \cdot \mathrm{adp}\right) \quad (82)$$

$$\mathrm{function\_22}\left(\mathrm{k}, \mathrm{atp}, \mathrm{amp}, \mathrm{keqak}, \mathrm{adp}\right) = \mathrm{k} \cdot \left(\mathrm{atp} \cdot \mathrm{amp} - \mathrm{keqak} \cdot \mathrm{adp} \cdot \mathrm{adp}\right) \quad (83)$$

Table 60: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k			1000000.000		☑
keqak			0.442		☑

7.19 Reaction vPGT

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

Name 3phosphoglycerate transport

Reaction equation

$$\mathrm{species\_23} \rightleftharpoons \mathrm{species\_7} \quad (84)$$

Reactant

Table 61: Properties of each reactant.

Id	Name	SBO
species_23	3phosphoglycerate	

Product

Table 62: Properties of each product.

Id	Name	SBO
species_7	3phosphoglycerate cytosol	

Kinetic Law

Derived unit contains undeclared units

$$v_{19} = \mathrm{k1} \cdot [\mathrm{species\_23}] - \mathrm{k2} \cdot [\mathrm{species\_7}] \quad (85)$$

Table 63: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1			1000000.0		☑
k2			1000000.0		☑

7.20 Reaction vANTI

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

Name gly3p dhap antiporter

Reaction equation

$$\mathrm{species\_22} + \mathrm{species\_8} \rightleftharpoons \mathrm{species\_9} + \mathrm{species\_17} \quad (86)$$

Reactants

Table 64: Properties of each reactant.

Id	Name	SBO
species_22	glycerol3phosphate	
species_8	dihydroxyacetonephosphate cytosol	

Products

Table 65: Properties of each product.

Id	Name	SBO
species_9	glycerol3phosphate cytosol	
species_17	dihydroxyacetonephosphate	

Kinetic Law

Derived unit contains undeclared units

$$v_{20} = \mathrm{k1} \cdot [\mathrm{species\_22}] \cdot [\mathrm{species\_8}] - \mathrm{k2} \cdot [\mathrm{species\_9}] \cdot [\mathrm{species\_17}] \quad (87)$$

Table 66: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1			1000000.0		☑
k2			1000000.0		☑

7.21 Reaction vGlyT

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

Name glycerol transport

Reaction equation

$$\mathrm{species\_24} \rightleftharpoons \mathrm{species\_27} \quad (88)$$

Reactant

Table 67: Properties of each reactant.

Id	Name	SBO
species_24	glycerol	

Product

Table 68: Properties of each product.

Id	Name	SBO
species_27	glycerol external	

Kinetic Law

Derived unit contains undeclared units

$$v_{21} = \mathrm{k1} \cdot [\mathrm{species\_24}] - \mathrm{k2} \cdot [\mathrm{species\_27}] \quad (89)$$

Table 69: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1			1000000.0		☑
k2			1000000.0		☑

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 species_1

Name pyruvate

Initial concentration $10\ \mathrm{mmol}\cdot\mathrm{ml}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_1} = v_{12} - v_{10} \tag{90}$$

8.2 Species species_2

Name adpc

Initial concentration $1.31652277625\ \mathrm{mmol}\cdot\mathrm{ml}^{-1}$

This species takes part in three reactions (as a reactant in vPK and as a product in vAU, vAKc).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_2} = v_{13} + 2\,v_{17} - v_{12} \tag{91}$$

8.3 Species species_3

Name atpc

Initial concentration $0.341738611875 \text{ mmol} \cdot \text{ml}^{-1}$

This species takes part in three reactions (as a reactant in vAU, vAKc and as a product in vPK).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_3} = v_{12} - v_{13} - v_{17} \tag{92}$$

8.4 Species species_4

Name phosphoenolpyruvate

Initial concentration $0 \text{ mmol} \cdot \text{ml}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_4} = v_{16} - v_{12} \tag{93}$$

8.5 Species species_5

Name 2phosphoglycerate

Initial concentration $0 \text{ mmol} \cdot \text{ml}^{-1}$

This species takes part in two reactions (as a reactant in vENO and as a product in vPGM).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_5} = v_{15} - v_{16} \tag{94}$$

8.6 Species species_6

Name ampc

Initial concentration $2.24173861188 \text{ mmol} \cdot \text{ml}^{-1}$

This species takes part in one reaction (as a reactant in vAKc).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_6} = -v_{17} \tag{95}$$

8.7 Species species_7

Name 3phosphoglycerate cytosol

Initial concentration $0 \text{ mmol} \cdot \text{ml}^{-1}$

This species takes part in two reactions (as a reactant in vPGM and as a product in vPGT).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_7} = v_{19} - v_{15} \tag{96}$$

8.8 Species species_8

Name dihydroxyacetonephosphate cytosol

Initial concentration $2.23134594788 \text{ mmol} \cdot \text{ml}^{-1}$

This species takes part in two reactions (as a reactant in vANTI and as a product in vGPO).

$$\frac{d}{dt}\text{species\_8} = v_9 - v_{20} \tag{97}$$

8.9 Species species_9

Name glycerol3phosphate cytosol

Initial concentration $2.76865405212 \text{ mmol} \cdot \text{ml}^{-1}$

This species takes part in two reactions (as a reactant in vGPO and as a product in vANTI).

$$\frac{d}{dt}\text{species\_9} = v_{20} - v_9 \tag{98}$$

8.10 Species species_10

Name glucose

Initial concentration $0 \text{ mmol} \cdot \text{ml}^{-1}$

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

$$\frac{d}{dt}\text{species\_10} = v_1 - v_2 \tag{99}$$

8.11 Species species_11

Name atpg

Initial concentration $0.240501857508 \text{ mmol} \cdot \text{ml}^{-1}$

This species takes part in six reactions (as a reactant in vHK, vPFK, vAKg and as a product in vPGK, vGK and as a modifier in vALD).

$$\frac{d}{dt}\text{species\_11} = v_{11} + v_{14} - v_2 - v_4 - v_{18} \tag{100}$$

8.12 Species species_12

Name adpg

Initial concentration $1.51899628498 \text{ mmol} \cdot \text{ml}^{-1}$

This species takes part in six reactions (as a reactant in vPGK, vGK and as a product in vHK, vPFK, vAKg and as a modifier in vALD).

$$\frac{d}{dt}\text{species\_12} = v_2 + v_4 + 2\,v_{18} - v_{11} - v_{14} \tag{101}$$

8.13 Species species_13

Name ampg

Initial concentration $4.24050185751 \text{ mmol} \cdot \text{ml}^{-1}$

This species takes part in two reactions (as a reactant in vAKg and as a modifier in vALD).

$$\frac{d}{dt}\text{species\_13} = -v_{18} \tag{102}$$

8.14 Species species_14

Name glucose6phosphate

Initial concentration $0.5 \text{ mmol} \cdot \text{ml}^{-1}$

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

$$\frac{d}{dt}\text{species\_14} = v_2 - v_3 \tag{103}$$

8.15 Species species_15

Name fructose6phosphate

Initial concentration $0.5 \text{ mmol} \cdot \text{ml}^{-1}$

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

$$\frac{d}{dt}\text{species\_15} = v_3 - v_4 \tag{104}$$

8.16 Species species_16

Name fructose16bisphosphate

Initial concentration $10 \text{ mmol} \cdot \text{ml}^{-1}$

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

$$\frac{d}{dt}\text{species\_16} = v_4 - v_5 \tag{105}$$

8.17 Species species_17

Name dihydroxyacetonephosphate

Initial concentration $8.47911460193\ \mathrm{mmol} \cdot \mathrm{ml}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t} \mathrm{species\_17} = v_5 + v_{20} - v_6 - v_8 \tag{106}$$

8.18 Species species_18

Name glyceraldehyde3phosphate

Initial concentration $2.5\ \mathrm{mmol} \cdot \mathrm{ml}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t} \mathrm{species\_18} = v_5 + v_6 - v_7 \tag{107}$$

8.19 Species species_19

Name nad

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

This species takes part in two reactions (as a reactant in vGAPDH and as a product in vGPDH).

$$\frac{\mathrm{d}}{\mathrm{d}t} \mathrm{species\_19} = v_8 - v_7 \tag{108}$$

8.20 Species species_20

Name nadh

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

This species takes part in two reactions (as a reactant in vGPDH and as a product in vGAPDH).

$$\frac{\mathrm{d}}{\mathrm{d}t} \mathrm{species\_20} = v_7 - v_8 \tag{109}$$

8.21 Species species_21

Name bisphosphoglycerate

Initial concentration $0.5\ \text{mmol} \cdot \text{ml}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_21} = v_7 - v_{11} \tag{110}$$

8.22 Species species_22

Name glycerol3phosphate

Initial concentration $10.5208853981\ \text{mmol} \cdot \text{ml}^{-1}$

This species takes part in three reactions (as a reactant in vGK, vANTI and as a product in vGPDH).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_22} = v_8 - v_{14} - v_{20} \tag{111}$$

8.23 Species species_23

Name 3phosphoglycerate

Initial concentration $0\ \text{mmol} \cdot \text{ml}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_23} = v_{11} - v_{19} \tag{112}$$

8.24 Species species_24

Name glycerol

Initial concentration $0\ \text{mmol} \cdot \text{ml}^{-1}$

This species takes part in two reactions (as a reactant in vGlyT and as a product in vGK).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_24} = v_{14} - v_{21} \tag{113}$$

8.25 Species species_25

Name glucose external

Initial concentration $5\ \text{mmol} \cdot \text{ml}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_25} = 0 \tag{114}$$

8.26 Species species_26

Name pyruvate external

Initial concentration $0 \text{ mmol} \cdot \text{ml}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_26} = 0 \tag{115}$$

8.27 Species species_27

Name glycerol external

Initial concentration $0 \text{ mmol} \cdot \text{ml}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{species\_27} = 0 \tag{116}$$

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