SBML Model Report

Model name: “Costa2014 - Computational Model of L. lactis Metabolism”

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1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by the following two authors: Audald Lloret i Villas[1] and Rafael Costa[2] at March 26th 2015 at 3:31 p. m. and last time modified at March 26th 2015 at 4:41 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	2
species types	0	species	26
events	0	constraints	0
reactions	21	function definitions	21
global parameters	0	unit definitions	1
rules	0	initial assignments	0

Model Notes

Costa2014 - Computational Model of L. lactisMetabolism

This model is described in the article:An extended dynamic model of Lactococcus lactis metabolism for mannitol and 2,3-butanediol production.Costa RS, Hartmann A, Gaspar P, Neves AR, Vinga S.Mol Biosyst 2014 Mar; 10(3): 628-639

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Abstract:

Biomedical research and biotechnological production are greatly benefiting from the results provided by the development of dynamic models of microbial metabolism. Although several kinetic models of Lactococcus lactis (a Lactic Acid Bacterium (LAB) commonly used in the dairy industry) have been developed so far, most of them are simplified and focus only on specific metabolic pathways. Therefore, the application of mathematical models in the design of an engineering strategy for the production of industrially important products by L. lactis has been very limited. In this work, we extend the existing kinetic model of L. lactis central metabolism to include industrially relevant production pathways such as mannitol and 2,3-butanediol. In this way, we expect to study the dynamics of metabolite production and make predictive simulations in L. lactis. We used a system of ordinary differential equations (ODEs) with approximate Michaelis-Menten-like kinetics for each reaction, where the parameters were estimated from multivariate time-series metabolite concentrations obtained by our team through in vivo Nuclear Magnetic Resonance (NMR). The results show that the model captures observed transient dynamics when validated under a wide range of experimental conditions. Furthermore, we analyzed the model using global perturbations, which corroborate experimental evidence about metabolic responses upon enzymatic changes. These include that mannitol production is very sensitive to lactate dehydrogenase (LDH) in the wild type (W.T.) strain, and to mannitol phosphoenolpyruvate: a phosphotransferase system (PTS(Mtl)) in a LDH mutant strain. LDH reduction has also a positive control on 2,3-butanediol levels. Furthermore, it was found that overproduction of mannitol-1-phosphate dehydrogenase (MPD) in a LDH/PTS(Mtl) deficient strain can increase the mannitol levels. The results show that this model has prediction capability over new experimental conditions and offers promising possibilities to elucidate the effect of alterations in the main metabolism of L. lactis, with application in strain optimization.

2 Unit Definitions

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

2.1 Unit `substance`

Name substance

Definition mmol

2.2 Unit volume

Notes Litre is the predefined SBML unit for volume.

Definition l

2.3 Unit area

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

Definition m^2

2.4 Unit length

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

Definition m

2.5 Unit time

Notes Second is the predefined SBML unit for time.

Definition s

3 Compartments

This model contains two compartments.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
compartment_1	Intracellular		3	0.047	l	☑	
compartment_2	Extracellular		3	1	litre	☑	

3.1 Compartment compartment_1

This is a three dimensional compartment with a constant size of 0.047 litre.

Name Intracellular

3.2 Compartment compartment_2

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

Name Extracellular

4 Species

This model contains 26 species. Section 7 provides further details and the derived rates of change of each species.

Table 3: Properties of each species.

Id	Name	Compartment	Derived Unit	Constant	Boundary Condition
G6P	G6P	compartment_1	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
ATP	ATP	compartment_1	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
ADP	ADP	compartment_1	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Pint	Pint	compartment_1	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
F6P	F6P	compartment_1	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
FBP	FBP	compartment_1	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
G3P	G3P	compartment_1	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
BPG	BPG	compartment_1	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
PEP	PEP	compartment_1	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
NAD	NAD	compartment_1	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
NADH	NADH	compartment_1	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
PYR	PYR	compartment_1	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
AcetCoA	AcetCoA	compartment_1	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Acetoin	Acetoin	compartment_1	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Mannitol	Mannitol	compartment_1	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Mannitol1Phosphate	Mannitol1Phosphate	compartment_1	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
CoA	CoA	compartment_1	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Pext	Pext	compartment_2	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Lactate	Lactate	compartment_2	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Ethanol	Ethanol	compartment_2	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Acetate	Acetate	compartment_2	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Butanediol	Butanediol	compartment_2	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟

Id	Name	Compartment	Derived Unit	Constant	Boundary Condition
Glucose	Glucose	compartment_2	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Acetoin_Ext	Acetoin_Ext	compartment_2	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Mannitol_Ext	Mannitol_Ext	compartment_2	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Formate	Formate	compartment_2	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	⊟	⊟

5 Function definitions

This is an overview of 21 function definitions.

5.1 Function definition `function_4_PTS_Glc`

Name function_4_PTS_Glc

Arguments [FBP], [G6P], [Glucose], [PEP], [PYR], [Pint], Vmax_PTS_Glc, kaPint_PTS_Glc, kiFBP_PTS_Glc, kmG6P_PTS_Glc, kmGlucose_PTS_Glc, kmPEP_PTS_Glc, kmPYR_PTS_Glc

Mathematical Expression

$$\frac{\frac{[\text{Pint}]}{[\text{Pint}]+\text{kaPint\_PTS\_Glc}} \cdot \frac{\text{kiFBP\_PTS\_Glc}}{[\text{FBP}]+\text{kiFBP\_PTS\_Glc}} \cdot \text{Vmax\_PTS\_Glc} \cdot \frac{[\text{Glucose}]}{\text{kmGlucose\_PTS\_Glc}} \cdot \frac{[\text{PEP}]}{\text{kmPEP\_PTS\_Glc}}}{\left(1+\frac{[\text{Glucose}]}{\text{kmGlucose\_PTS\_Glc}}\right) \cdot \left(1+\frac{[\text{PEP}]}{\text{kmPEP\_PTS\_Glc}}\right) + \left(1+\frac{[\text{G6P}]}{\text{kmG6P\_PTS\_Glc}}\right) \cdot \left(1+\frac{[\text{PYR}]}{\text{kmPYR\_PTS\_Glc}}\right) - 1} \tag{1}$$

5.2 Function definition `function_4_ATPase`

Name function_4_ATPase

Arguments [ATP], Vmax_ATPase, kmATP_ATPase, nATPase

Mathematical Expression

$$\text{Vmax\_ATPase} \cdot \frac{\left(\frac{[\text{ATP}]}{\text{kmATP\_ATPase}}\right)^{\text{nATPase}}}{\left(\frac{[\text{ATP}]}{\text{kmATP\_ATPase}}\right)^{\text{nATPase}} + 1} \tag{2}$$

5.3 Function definition `function_4_P_transp`

Name function_4_P_transp

Arguments [ADP], [ATP], [Pext], [Pint], Vmax_Ptransport, kiPint_Ptransport, kmADP_Ptransport, kmATP_Ptransport, kmPext_Ptransport, kmPint_Ptransport

Mathematical Expression

$$\frac{\frac{\text{kiPint\_Ptransport}}{[\text{Pint}]+\text{kiPint\_Ptransport}} \cdot \text{Vmax\_Ptransport} \cdot \frac{[\text{ATP}]}{\text{kmATP\_Ptransport}} \cdot \frac{[\text{Pext}]}{\text{kmPext\_Ptransport}}}{\left(1+\frac{[\text{Pext}]}{\text{kmPext\_Ptransport}}\right) \cdot \left(1+\frac{[\text{ATP}]}{\text{kmATP\_Ptransport}}\right) + \left(1+\frac{[\text{Pint}]}{\text{kmPint\_Ptransport}} + \left(\frac{[\text{Pint}]}{\text{kmPint\_Ptransport}}\right)^2\right) \cdot \left(1+\frac{[\text{ADP}]}{\text{kmADP\_Ptransport}}\right)} \tag{3}$$

5.4 Function definition function_4_PGI

Name function_4_PGI

Arguments [F6P], [G6P], Keq_PGI, Vmax_PGI, kmF6P_PGI, kmG6P_PGI

Mathematical Expression

$$\frac{\text{Vmax\_PGI} \cdot \frac{[\text{G6P}]}{\text{kmG6P\_PGI}} - \frac{\text{Vmax\_PGI}}{\text{Keq\_PGI}} \cdot \frac{[\text{F6P}]}{\text{kmG6P\_PGI}}}{1 + \frac{[\text{G6P}]}{\text{kmG6P\_PGI}} + \frac{[\text{F6P}]}{\text{kmF6P\_PGI}}} \tag{4}$$

5.5 Function definition function_4_PFK

Name function_4_PFK

Arguments [ADP], [ATP], [F6P], [FBP], Vmax_PFK, kmADP_PFK, kmATP_PFK, kmF6P_PFK, kmFBP_PFK

Mathematical Expression

$$\frac{\text{Vmax\_PFK} \cdot \frac{[\text{F6P}]}{\text{kmF6P\_PFK}} \cdot \frac{[\text{ATP}]}{\text{kmATP\_PFK}}}{\left(1 + \frac{[\text{F6P}]}{\text{kmF6P\_PFK}}\right) \cdot \left(1 + \frac{[\text{ATP}]}{\text{kmATP\_PFK}}\right) + \left(1 + \frac{[\text{FBP}]}{\text{kmFBP\_PFK}}\right) \cdot \left(1 + \frac{[\text{ADP}]}{\text{kmADP\_PFK}}\right) - 1} \tag{5}$$

5.6 Function definition function_4_FBA

Name function_4_FBA

Arguments [FBP], [G3P], Keq_FBA, Vmax_FBA, kmFBP_FBA, kmG3P_FBA

Mathematical Expression

$$\frac{\text{Vmax\_FBA} \cdot \frac{[\text{FBP}]}{\text{kmFBP\_FBA}} - \frac{\text{Vmax\_FBA}}{\text{Keq\_FBA}} \cdot \frac{[\text{G3P}]^2}{\text{kmFBP\_FBA}}}{1 + \frac{[\text{FBP}]}{\text{kmFBP\_FBA}} + \frac{[\text{G3P}]}{\text{kmG3P\_FBA}} + \left(\frac{[\text{G3P}]}{\text{kmG3P\_FBA}}\right)^2} \tag{6}$$

5.7 Function definition function_4_GAPDH

Name function_4_GAPDH

Arguments [BPG], [G3P], Keq_GAPDH, [NAD], [NADH], [Pint], Vmax_GAPDH, kmBPG_GAPDH, kmG3P_GAPDH, kmNADH_GAPDH, kmNAD_GAPDH, kmPint_GAPDH

Mathematical Expression

$$\frac{\text{Vmax\_GAPDH} \cdot \frac{[\text{G3P}]}{\text{kmG3P\_GAPDH}} \cdot \frac{[\text{NAD}]}{\text{kmNAD\_GAPDH}} \cdot \frac{[\text{Pint}]}{\text{kmPint\_GAPDH}} - \frac{\text{Vmax\_GAPDH}}{\text{Keq\_GAPDH}} \cdot \frac{[\text{BPG}]}{\text{kmG3P\_GAPDH}} \cdot \frac{[\text{NADH}]}{\text{kmNAD\_GAPDH}} \cdot \frac{1}{\text{kmPint\_G}}}{\left(1 + \frac{[\text{G3P}]}{\text{kmG3P\_GAPDH}}\right) \cdot \left(1 + \frac{[\text{Pint}]}{\text{kmPint\_GAPDH}}\right) \cdot \left(1 + \frac{[\text{NAD}]}{\text{kmNAD\_GAPDH}}\right) + \left(1 + \frac{[\text{BPG}]}{\text{kmBPG\_GAPDH}}\right) \cdot \left(1 + \frac{[\text{NADH}]}{\text{kmNADH\_GAPDH}}\right)} \tag{7}$$

5.8 Function definition function_4_ENO

Name function_4_ENO

Arguments [ADP], [ATP], [BPG], Keq_ENO, [PEP], Vmax_ENO, kmADP_ENO, kmATP_ENO, kmBPG_ENO, kmPEP_ENO

Mathematical Expression

$$\frac{\text{Vmax\_ENO} \cdot \frac{[\text{BPG}]}{\text{kmBPG\_ENO}} \cdot \frac{[\text{ADP}]}{\text{kmADP\_ENO}} - \frac{\text{Vmax\_ENO}}{\text{Keq\_ENO}} \cdot \frac{[\text{PEP}]}{\text{kmBPG\_ENO}} \cdot \frac{[\text{ATP}]}{\text{kmADP\_ENO}}}{\left(1 + \frac{[\text{BPG}]}{\text{kmBPG\_ENO}}\right) \cdot \left(1 + \frac{[\text{ADP}]}{\text{kmADP\_ENO}}\right) + \left(1 + \frac{[\text{PEP}]}{\text{kmPEP\_ENO}}\right) \cdot \left(1 + \frac{[\text{ATP}]}{\text{kmATP\_ENO}}\right) - 1} \tag{8}$$

5.9 Function definition function_4_PYK

Name function_4_PYK

Arguments [ADP], [ATP], [FBP], [PEP], [PYR], [Pint], Vmax_PYK, kaFBP_PYK, kiPint_PYK, kmADP_PYK, kmATP_PYK, kmPEP_PYK, kmPYR_PYK, nPYK

Mathematical Expression

$$\frac{\frac{[\text{FBP}]}{[\text{FBP}]+\text{kaFBP\_PYK}} \cdot \frac{\text{kiPint\_PYK}^{\text{nPYK}}}{[\text{Pint}]^{\text{nPYK}}+\text{kiPint\_PYK}^{\text{nPYK}}} \cdot \text{Vmax\_PYK} \cdot \frac{[\text{ADP}]}{\text{kmADP\_PYK}} \cdot \frac{[\text{PEP}]}{\text{kmPEP\_PYK}}}{\left(1 + \frac{[\text{ADP}]}{\text{kmADP\_PYK}}\right) \cdot \left(1 + \frac{[\text{PEP}]}{\text{kmPEP\_PYK}}\right) + \left(1 + \frac{[\text{ATP}]}{\text{kmATP\_PYK}}\right) \cdot \left(1 + \frac{[\text{PYR}]}{\text{kmPYR\_PYK}}\right) - 1} \tag{9}$$

5.10 Function definition function_4_LDH

Name function_4_LDH

Arguments [FBP], [Lactate], [NAD], [NADH], [PYR], [Pint], Vmax_LDH, kaFBP_LDH, kiPint_LDH, kmLactate_LDH, kmNADH_LDH, kmNAD_LDH, kmPYR_LDH

Mathematical Expression

$$\frac{\frac{[\text{FBP}]}{[\text{FBP}]+\text{kaFBP\_LDH}} \cdot \frac{\text{kiPint\_LDH}}{[\text{Pint}]+\text{kiPint\_LDH}} \cdot \text{Vmax\_LDH} \cdot \frac{[\text{PYR}]}{\text{kmPYR\_LDH}} \cdot \frac{[\text{NADH}]}{\text{kmNADH\_LDH}}}{\left(1 + \frac{[\text{PYR}]}{\text{kmPYR\_LDH}}\right) \cdot \left(1 + \frac{[\text{NADH}]}{\text{kmNADH\_LDH}}\right) + \left(1 + \frac{[\text{Lactate}]}{\text{kmLactate\_LDH}}\right) \cdot \left(1 + \frac{[\text{NAD}]}{\text{kmNAD\_LDH}}\right) - 1} \tag{10}$$

5.11 Function definition function_4_PFL

Name function_4_PFL

Arguments [AcetCoA], [CoA], [Formate], [G3P], Keq_PFL, KmCoA_PFL, [PYR], Vmax_PFL, kiG3P_PFL, kmAcetCoA_PFL, kmFormate_PFL, kmPYR_PFL

Mathematical Expression

$$\frac{\frac{\text{kiG3P\_PFL}}{\text{[G3P]+kiG3P\_PFL}} \cdot \left(\text{Vmax\_PFL} \cdot \frac{\text{[PYR]}}{\text{kmPYR\_PFL}} \cdot \frac{\text{[CoA]}}{\text{KmCoA\_PFL}} - \frac{\text{Vmax\_PFL}}{\text{Keq\_PFL}} \cdot \frac{\text{[AcetCoA]}}{\text{kmPYR\_PFL}} \cdot \frac{\text{[Formate]}}{\text{KmCoA\_PFL}}\right)}{\left(1 + \frac{\text{[PYR]}}{\text{kmPYR\_PFL}}\right) \cdot \left(1 + \frac{\text{[CoA]}}{\text{KmCoA\_PFL}}\right) + \left(1 + \frac{\text{[AcetCoA]}}{\text{kmAcetCoA\_PFL}}\right) \cdot \left(1 + \frac{\text{[Formate]}}{\text{kmFormate\_PFL}}\right) - 1} \tag{11}$$

5.12 Function definition `function_4_AE`

Name function_4_AE

Arguments [ATP], [AcetCoA], [CoA], [Ethanol], [NAD], [NADH], Vmax_AE, kiATP_AE, kmAcetCoA_AE, kmCoA_AE, kmEthanol_AE, kmNADH_AE, kmNAD_AE

Mathematical Expression

$$\frac{\frac{\text{kiATP\_AE}}{\text{[ATP]+kiATP\_AE}} \cdot \text{Vmax\_AE} \cdot \frac{\text{[AcetCoA]}}{\text{kmAcetCoA\_AE}} \cdot \left(\frac{\text{[NADH]}}{\text{kmNADH\_AE}}\right)^2}{\left(1 + \frac{\text{[NADH]}}{\text{kmNADH\_AE}} + \left(\frac{\text{[NADH]}}{\text{kmNADH\_AE}}\right)^2\right) \cdot \left(1 + \frac{\text{[AcetCoA]}}{\text{kmAcetCoA\_AE}}\right) + \left(1 + \frac{\text{[Ethanol]}}{\text{kmEthanol\_AE}}\right) \cdot \left(1 + \frac{\text{[CoA]}}{\text{kmCoA\_AE}}\right) \cdot \left(1 + \frac{\text{[NAD]}}{\text{kmNAD\_A}}\right.} \tag{12}$$

5.13 Function definition `function_4_ACK`

Name function_4_ACK

Arguments [ADP], [ATP], [AcetCoA], [Acetate], [CoA], Vmax_ACK, kmADP_ACK, kmATP_ACK, kmAcetCoA_ACK, kmAcetate_ACK, kmCoA_ACK

Mathematical Expression

$$\frac{\text{Vmax\_ACK} \cdot \frac{\text{[AcetCoA]}}{\text{kmAcetCoA\_ACK}} \cdot \frac{\text{[ADP]}}{\text{kmADP\_ACK}}}{\left(1 + \frac{\text{[AcetCoA]}}{\text{kmAcetCoA\_ACK}}\right) \cdot \left(1 + \frac{\text{[ADP]}}{\text{kmADP\_ACK}}\right) + \left(1 + \frac{\text{[Acetate]}}{\text{kmAcetate\_ACK}}\right) \cdot \left(1 + \frac{\text{[ATP]}}{\text{kmATP\_ACK}}\right) \cdot \left(1 + \frac{\text{[CoA]}}{\text{kmCoA\_ACK}}\right) - 1} \tag{13}$$

5.14 Function definition `function_4_ALS`

Name function_4_ALS

Arguments [Acetoin], Keq_ALS, [PYR], Vmax_ALS, kmAcetoin_ALS, kmPYR_ALS

Mathematical Expression

$$\frac{\text{Vmax\_ALS} \cdot \left(\frac{\text{[PYR]}}{\text{kmPYR\_ALS}}\right)^2 - \frac{\text{Vmax\_ALS}}{\text{Keq\_ALS}} \cdot \frac{\text{[Acetoin]}}{\text{kmPYR\_ALS}}}{1 + \frac{\text{[PYR]}}{\text{kmPYR\_ALS}} + \left(\frac{\text{[PYR]}}{\text{kmPYR\_ALS}}\right)^2 + 1 + \frac{\text{[Acetoin]}}{\text{kmAcetoin\_ALS}} - 1} \tag{14}$$

5.15 Function definition function_4_BDH

Name function_4_BDH

Arguments [Acetoin], [Butanediol], Keq_BDH, [NAD], [NADH], Vmax_BDH, kmAcetoin_BDH, kmButanediol_BDH, kmNADH_BDH, kmNAD_BDH

Mathematical Expression

$$\frac{\text{Vmax\_BDH} \cdot \frac{[\text{Acetoin}]}{\text{kmAcetoin\_BDH}} \cdot \frac{[\text{NADH}]}{\text{kmNADH\_BDH}} - \frac{\text{Vmax\_BDH}}{\text{Keq\_BDH}} \cdot \frac{[\text{Butanediol}]}{\text{kmAcetoin\_BDH}} \cdot \frac{[\text{NAD}]}{\text{kmNADH\_BDH}}}{\left(1 + \frac{[\text{Acetoin}]}{\text{kmAcetoin\_BDH}}\right) \cdot \left(1 + \frac{[\text{NADH}]}{\text{kmNADH\_BDH}}\right) + \left(1 + \frac{[\text{Butanediol}]}{\text{kmButanediol\_BDH}}\right) \cdot \left(1 + \frac{[\text{NAD}]}{\text{kmNAD\_BDH}}\right) - 1} \tag{15}$$

5.16 Function definition function_4_MPD

Name function_4_MPD

Arguments [F6P], Keq_MPD, [Mannitol1Phosphate], [NAD], [NADH], Vmax_MPD, kiF6P_MPD, kmF6P_MPD, kmMannitol1Phoshate_MPD, kmNADH_MPD, kmNAD_MPD

Mathematical Expression

$$\frac{\frac{\text{kiF6P\_MPD}}{[\text{F6P}]+\text{kiF6P\_MPD}} \cdot \left(\text{Vmax\_MPD} \cdot \frac{[\text{F6P}]}{\text{kmF6P\_MPD}} \cdot \frac{[\text{NADH}]}{\text{kmNADH\_MPD}} - \frac{\text{Vmax\_MPD}}{\text{Keq\_MPD}} \cdot \frac{[\text{Mannitol1Phosphate}]}{\text{kmF6P\_MPD}} \cdot \frac{[\text{NAD}]}{\text{kmNADH\_MPD}}\right)}{\left(1 + \frac{[\text{F6P}]}{\text{kmF6P\_MPD}}\right) \cdot \left(1 + \frac{[\text{NADH}]}{\text{kmNADH\_MPD}}\right) + \left(1 + \frac{[\text{Mannitol1Phosphate}]}{\text{kmMannitol1Phoshate\_MPD}}\right) \cdot \left(1 + \frac{[\text{NAD}]}{\text{kmNAD\_MPD}}\right) - 1} \tag{16}$$

5.17 Function definition function_4_MP

Name function_4_MP

Arguments [Mannitol], [Mannitol1Phosphate], Vmax_MP, kmMannitol1Phosphate_MP, kmMannitol_MP

Mathematical Expression

$$\frac{\text{Vmax\_MP} \cdot \frac{[\text{Mannitol1Phosphate}]}{\text{kmMannitol1Phosphate\_MP}}}{1 + \frac{[\text{Mannitol1Phosphate}]}{\text{kmMannitol1Phosphate\_MP}} + 1 + \frac{[\text{Mannitol}]}{\text{kmMannitol\_MP}} - 1} \tag{17}$$

5.18 Function definition function_4_PTS_Man

Name function_4_PTS_Man

Arguments [Mannitol1Phosphate], [Mannitol_Ext], [PEP], [PYR], Vmax_PTS_Man, kmMannitol1Phosphate_PTS_M kmMannitolExt_PTS_Man, kmPEP_PTS_Man, kmPYR_PTS_Man

Mathematical Expression

$$\frac{\text{Vmax\_PTS\_Man} \cdot \frac{[\text{Mannitol\_Ext}]}{\text{kmMannitolExt\_PTS\_Man}} \cdot \frac{[\text{PEP}]}{\text{kmPEP\_PTS\_Man}}}{\left(1 + \frac{[\text{Mannitol\_Ext}]}{\text{kmMannitolExt\_PTS\_Man}}\right) \cdot \left(1 + \frac{[\text{PEP}]}{\text{kmPEP\_PTS\_Man}}\right) + \left(1 + \frac{[\text{Mannitol1Phosphate}]}{\text{kmMannitol1Phosphate\_PTS\_Man}}\right) \cdot \left(1 + \frac{[\text{PYR}]}{\text{kmPYR\_PTS\_Man}}\right) - 1} \tag{18}$$

5.19 Function definition function_4_Acetoin_transp

Name function_4_Acetoin_transp

Arguments [Acetoin], [Acetoin_Ext], Vmax_Acetoin_transp, kmAcetoin_Acetoin_transp, kmAcetoin_Ext_Acetoin_t

Mathematical Expression

$$\frac{\text{Vmax\_Acetoin\_transp} \cdot \frac{[\text{Acetoin}]}{\text{kmAcetoin\_Acetoin\_transp}}}{1 + \frac{[\text{Acetoin}]}{\text{kmAcetoin\_Acetoin\_transp}} + \frac{[\text{Acetoin\_Ext}]}{\text{kmAcetoin\_Ext\_Acetoin\_transp}}} \tag{19}$$

5.20 Function definition function_4_Mannitol_transp

Name function_4_Mannitol_transp

Arguments [Mannitol], [Mannitol_Ext], Vmax_Mannitol_transp, kmMannitol_Ext_Mannitol_transp, kmMannitol_Mannitol_transp

Mathematical Expression

$$\frac{\text{Vmax\_Mannitol\_transp} \cdot \frac{[\text{Mannitol}]}{\text{kmMannitol\_Mannitol\_transp}}}{1 + \frac{[\text{Mannitol}]}{\text{kmMannitol\_Mannitol\_transp}} + \frac{[\text{Mannitol\_Ext}]}{\text{kmMannitol\_Ext\_Mannitol\_transp}}} \tag{20}$$

5.21 Function definition function_4_FBPase

Name function_4_FBPase

Arguments [F6P], [FBP], [Pint], Vmax_FBPase, kmF6P_FBPase, kmFBP_FBPase, kmPint_FBPase

Mathematical Expression

$$\frac{\text{Vmax\_FBPase} \cdot \frac{[\text{FBP}]}{\text{kmFBP\_FBPase}}}{\frac{[\text{FBP}]}{\text{kmFBP\_FBPase}} + \left(1 + \frac{[\text{F6P}]}{\text{kmF6P\_FBPase}}\right) \cdot \left(1 + \frac{[\text{Pint}]}{\text{kmPint\_FBPase}}\right)} \tag{21}$$

6 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 4: Overview of all reactions

№	Id	Name	Reaction Equation	SBO
1	re12	PTS_Glc	$\text{Glucose} + \text{PEP} \xrightarrow{\text{FBP, Pint, FBP, G6P, Glucose, PEP, PYR, Pint}} \text{G6P} + \text{PYR}$	
2	re13	ATPase	$\text{ATP} \xrightarrow{\text{ATP}} \text{ADP} + \text{Pint}$	
3	re14	P_transp	$\text{Pext} + \text{ATP} \xrightarrow{\text{Pint, ADP, ATP, Pext, Pint}} 2\,\text{Pint} + \text{ADP}$	
4	re15	PGI	$\text{G6P} \xrightleftharpoons{\text{F6P, G6P}} \text{F6P}$	
5	re16	PFK	$\text{F6P} + \text{ATP} \xrightarrow{\text{ADP, ATP, F6P, FBP}} \text{FBP} + \text{ADP}$	
6	re17	FBA	$\text{FBP} \xrightleftharpoons{\text{FBP, G3P}} 2\,\text{G3P}$	
7	re18	GAPDH	$\text{G3P} + \text{Pint} + \text{NAD} \xrightleftharpoons{\text{BPG, G3P, NAD, NADH, Pint}} \text{BPG} + \text{NADH}$	
8	re20	ENO	$\text{BPG} + \text{ADP} \xrightleftharpoons{\text{ADP, ATP, BPG, PEP}} \text{PEP} + \text{ATP}$	
9	re21	PYK	$\text{PEP} + \text{ADP} \xrightarrow{\text{FBP, Pint, ADP, ATP, FBP, PEP, PYR, Pint}} \text{PYR} + \text{ATP}$	
10	re22	LDH	$\text{PYR} + \text{NADH} \xrightarrow{\text{FBP, Pint, FBP, Lactate, NAD, NADH, PYR, Pint}} \text{Lactate} + \text{NAD}$	
11	re23	PDH	$\text{PYR} + \text{CoA} \xrightleftharpoons{\text{G3P, AcetCoA, CoA, Formate, G3P, PYR}} \text{AcetCoA} + \text{Formate}$	

№	Id	Name	Reaction Equation	SBO
12	re24	AE	$\mathrm{AcetCoA} + 2\,\mathrm{NADH} \xrightarrow{\mathrm{ATP,\ ATP,\ AcetCoA,\ CoA,\ Ethanol,\ NAD,\ NADH}} \mathrm{Ethanol} + 2\,\mathrm{NAD} + \mathrm{CoA}$	
13	re25	AC	$\mathrm{AcetCoA} + \mathrm{ADP} \xrightarrow{\mathrm{ADP,\ ATP,\ AcetCoA,\ Acetate,\ CoA}} \mathrm{Acetate} + \mathrm{ATP} + \mathrm{CoA}$	
14	re26	PA	$2\,\mathrm{PYR} \xrightleftharpoons{\mathrm{Acetoin,\ PYR}} \mathrm{Acetoin}$	
15	re27	AB	$\mathrm{Acetoin} + \mathrm{NADH} \xrightleftharpoons{\mathrm{Acetoin,\ Butanediol,\ NAD,\ NADH}} \mathrm{Butanediol} + \mathrm{NAD}$	
16	re28	MPD	$\mathrm{F6P} + \mathrm{NADH} \xrightleftharpoons{\mathrm{F6P,\ F6P,\ Mannitol1Phosphate,\ NAD,\ NADH}} \mathrm{Mannitol1Phosphate} + \mathrm{NAD}$	
17	re29	MP	$\mathrm{Mannitol1Phosphate} \xrightarrow{\mathrm{Mannitol,\ Mannitol1Phosphate}} \mathrm{Mannitol}$	
18	re30	PTS_Man	$\mathrm{Mannitol\_Ext} + \mathrm{PEP} \xrightarrow{\mathrm{Mannitol1Phosphate,\ Mannitol\_Ext,\ PEP,\ PYR}} \mathrm{Mannitol1Phosph} + \mathrm{PYR}$	
19	re31	Acetoin_transp	$\mathrm{Acetoin} \xrightarrow{\mathrm{Acetoin,\ Acetoin\_Ext}} \mathrm{Acetoin\_Ext}$	
20	re32	Mannitol_transp	$\mathrm{Mannitol} \xrightarrow{\mathrm{Mannitol,\ Mannitol\_Ext}} \mathrm{Mannitol\_Ext}$	
21	re33	FBPase	$\mathrm{FBP} \xrightarrow{\mathrm{F6P,\ FBP,\ Pint}} \mathrm{F6P} + \mathrm{Pint}$	

6.1 Reaction re12

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

Name PTS_Glc

Reaction equation

$$\text{Glucose} + \text{PEP} \xrightarrow{\text{FBP, Pint, FBP, G6P, Glucose, PEP, PYR, Pint}} \text{G6P} + \text{PYR} \qquad (22)$$

Reactants

Table 5: Properties of each reactant.

Id	Name	SBO
Glucose	Glucose	
PEP	PEP	

Modifiers

Table 6: Properties of each modifier.

Id	Name	SBO
FBP	FBP	
Pint	Pint	
FBP	FBP	
G6P	G6P	
Glucose	Glucose	
PEP	PEP	
PYR	PYR	
Pint	Pint	

Products

Table 7: Properties of each product.

Id	Name	SBO
G6P	G6P	
PYR	PYR	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \text{function\_4\_PTS\_Glc}([\text{FBP}], [\text{G6P}], [\text{Glucose}], [\text{PEP}], [\text{PYR}], [\text{Pint}], \text{Vmax\_PTS\_Glc}, \text{kaPint\_PTS\_Glc}, \text{kiFBP\_PTS\_Glc}, \text{kmG6P\_PTS\_Glc}, \text{kmGlucose\_PTS\_Glc}, \text{kmPEP\_PTS\_Glc}, \text{kmPYR\_PTS\_Glc}) \quad (23)$$

$$\begin{aligned} &\text{function\_4\_PTS\_Glc}([\text{FBP}], [\text{G6P}], [\text{Glucose}], [\text{PEP}], [\text{PYR}], [\text{Pint}], \\ &\text{Vmax\_PTS\_Glc}, \text{kaPint\_PTS\_Glc}, \text{kiFBP\_PTS\_Glc}, \text{kmG6P\_PTS\_Glc}, \\ &\text{kmGlucose\_PTS\_Glc}, \text{kmPEP\_PTS\_Glc}, \text{kmPYR\_PTS\_Glc}) \\ &= \frac{\frac{[\text{Pint}]}{[\text{Pint}]+\text{kaPint\_PTS\_Glc}} \cdot \frac{\text{kiFBP\_PTS\_Glc}}{[\text{FBP}]+\text{kiFBP\_PTS\_Glc}} \cdot \text{Vmax\_PTS\_Glc} \cdot \frac{[\text{Glucose}]}{\text{kmGlucose\_PTS\_Glc}} \cdot \frac{[\text{PEP}]}{\text{kmPEP\_PTS\_Glc}}}{\left(1 + \frac{[\text{Glucose}]}{\text{kmGlucose\_PTS\_Glc}}\right) \cdot \left(1 + \frac{[\text{PEP}]}{\text{kmPEP\_PTS\_Glc}}\right) + \left(1 + \frac{[\text{G6P}]}{\text{kmG6P\_PTS\_Glc}}\right) \cdot \left(1 + \frac{[\text{PYR}]}{\text{kmPYR\_PTS\_Glc}}\right) - 1} \end{aligned} \quad (24)$$

Table 8: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax_PTS_Glc	Vmax_PTS_Glc		3.711		☑
kaPint_PTS_Glc	kaPint_PTS_Glc		0.071		☑
kiFBP_PTS_Glc	kiFBP_PTS_Glc		1.169		☑
kmG6P_PTS_Glc	kmG6P_PTS_Glc		0.285		☑
kmGlucose_PTS_Glc	kmGlucose_PTS_Glc		0.049		☑
kmPEP_PTS_Glc	kmPEP_PTS_Glc		0.306		☑
kmPYR_PTS_Glc	kmPYR_PTS_Glc		1.960		☑

6.2 Reaction re13

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

Name ATPase

Reaction equation

$$\text{ATP} \xrightarrow{\text{ATP}} \text{ADP} + \text{Pint} \quad (25)$$

Reactant

Table 9: Properties of each reactant.

Id	Name	SBO
ATP	ATP	

Modifier

Table 10: Properties of each modifier.

Id	Name	SBO
ATP	ATP	

Products

Table 11: Properties of each product.

Id	Name	SBO
ADP	ADP	
Pint	Pint	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \mathrm{vol}\left(\mathrm{compartment\_1}\right) \cdot \mathrm{function\_4\_ATPase}\left([\mathrm{ATP}], \mathrm{Vmax\_ATPase}, \mathrm{kmATP\_ATPase}, \mathrm{nATPase}\right) \tag{26}$$

$$\mathrm{function\_4\_ATPase}\left([\mathrm{ATP}], \mathrm{Vmax\_ATPase}, \mathrm{kmATP\_ATPase}, \mathrm{nATPase}\right) = \mathrm{Vmax\_ATPase} \cdot \frac{\left(\frac{[\mathrm{ATP}]}{\mathrm{kmATP\_ATPase}}\right)^{\mathrm{nATPase}}}{\left(\frac{[\mathrm{ATP}]}{\mathrm{kmATP\_ATPase}}\right)^{\mathrm{nATPase}} + 1} \tag{27}$$

$$\mathrm{function\_4\_ATPase}\left([\mathrm{ATP}], \mathrm{Vmax\_ATPase}, \mathrm{kmATP\_ATPase}, \mathrm{nATPase}\right) = \mathrm{Vmax\_ATPase} \cdot \frac{\left(\frac{[\mathrm{ATP}]}{\mathrm{kmATP\_ATPase}}\right)^{\mathrm{nATPase}}}{\left(\frac{[\mathrm{ATP}]}{\mathrm{kmATP\_ATPase}}\right)^{\mathrm{nATPase}} + 1} \tag{28}$$

Table 12: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
`Vmax_ATPase`	Vmax_ATPase		3.290		☑
`kmATP_ATPase`	kmATP_ATPase		4.342		☑
`nATPase`	nATPase		3.000		☑

6.3 Reaction `re14`

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

Name P_transp

Reaction equation

$$\mathrm{Pext} + \mathrm{ATP} \xrightarrow{\mathrm{Pint,\ ADP,\ ATP,\ Pext,\ Pint}} 2\,\mathrm{Pint} + \mathrm{ADP} \tag{29}$$

Reactants

Table 13: Properties of each reactant.

Id	Name	SBO
`Pext`	Pext	
`ATP`	ATP	

Modifiers

Table 14: Properties of each modifier.

Id	Name	SBO
`Pint`	Pint	
`ADP`	ADP	
`ATP`	ATP	
`Pext`	Pext	
`Pint`	Pint	

Products

Table 15: Properties of each product.

Id	Name	SBO
`Pint`	Pint	
`ADP`	ADP	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \text{function\_4\_P\_transp}([\text{ADP}], [\text{ATP}], [\text{Pext}], [\text{Pint}], \text{Vmax\_Ptransport}, \text{kiPint\_Ptransport}, \text{kmADP\_Ptransport}, \text{kmATP\_Ptransport}, \text{kmPext\_Ptransport}, \text{kmPint\_Ptransport}) \tag{30}$$

$$\text{function\_4\_P\_transp}([\text{ADP}], [\text{ATP}], [\text{Pext}], [\text{Pint}], \text{Vmax\_Ptransport}, \text{kiPint\_Ptransport}, \text{kmADP\_Ptransport}, \text{kmATP\_Ptransport}, \text{kmPext\_Ptransport}, \text{kmPint\_Ptransport}) \tag{31}$$

$$= \frac{\frac{\text{kiPint\_Ptransport}}{[\text{Pint}]+\text{kiPint\_Ptransport}} \cdot \text{Vmax\_Ptransport} \cdot \frac{[\text{ATP}]}{\text{kmATP\_Ptransport}} \cdot \frac{[\text{Pext}]}{\text{kmPext\_Ptransport}}}{\left(1 + \frac{[\text{Pext}]}{\text{kmPext\_Ptransport}}\right) \cdot \left(1 + \frac{[\text{ATP}]}{\text{kmATP\_Ptransport}}\right) + \left(1 + \frac{[\text{Pint}]}{\text{kmPint\_Ptransport}} + \left(\frac{[\text{Pint}]}{\text{kmPint\_Ptransport}}\right)^2\right) \cdot \left(1 + \frac{[\text{ADP}]}{\text{kmADP\_Ptransport}}\right.}$$

Table 16: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
`Vmax_Ptransport`	Vmax_Ptransport		3.596		☑
`kiPint_Ptransport`	kiPint_Ptransport		0.561		☑
`kmADP_Ptransport`	kmADP_Ptransport		0.192		☑
`kmATP_Ptransport`	kmATP_Ptransport		0.523		☑
`kmPext_Ptransport`	kmPext_Ptransport		0.750		☑
`kmPint_Ptransport`	kmPint_Ptransport		0.303		☑

6.4 Reaction `re15`

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

Name PGI

Reaction equation

$$\text{G6P} \underset{\longleftarrow}{\overset{\text{F6P, G6P}}{\longrightarrow}} \text{F6P} \tag{32}$$

Reactant

Table 17: Properties of each reactant.

Id	Name	SBO
G6P	G6P	

Modifiers

Table 18: Properties of each modifier.

Id	Name	SBO
F6P	F6P	
G6P	G6P	

Product

Table 19: Properties of each product.

Id	Name	SBO
F6P	F6P	

Kinetic Law

Derived unit contains undeclared units

$$\begin{aligned} v_4 = {} & \text{vol}\left(\text{compartment\_1}\right) \\ & \cdot \text{function\_4\_PGI}\left([\text{F6P}], [\text{G6P}], \text{Keq\_PGI}, \text{Vmax\_PGI}, \text{kmF6P\_PGI}, \text{kmG6P\_PGI}\right) \end{aligned} \tag{33}$$

$$\begin{aligned} & \text{function\_4\_PGI}\left([\text{F6P}], [\text{G6P}], \text{Keq\_PGI}, \text{Vmax\_PGI}, \text{kmF6P\_PGI}, \text{kmG6P\_PGI}\right) \\ & = \frac{\text{Vmax\_PGI} \cdot \frac{[\text{G6P}]}{\text{kmG6P\_PGI}} - \frac{\text{Vmax\_PGI}}{\text{Keq\_PGI}} \cdot \frac{[\text{F6P}]}{\text{kmG6P\_PGI}}}{1 + \frac{[\text{G6P}]}{\text{kmG6P\_PGI}} + \frac{[\text{F6P}]}{\text{kmF6P\_PGI}}} \end{aligned} \tag{34}$$

$$\begin{aligned} & \text{function\_4\_PGI}\left([\text{F6P}], [\text{G6P}], \text{Keq\_PGI}, \text{Vmax\_PGI}, \text{kmF6P\_PGI}, \text{kmG6P\_PGI}\right) \\ & = \frac{\text{Vmax\_PGI} \cdot \frac{[\text{G6P}]}{\text{kmG6P\_PGI}} - \frac{\text{Vmax\_PGI}}{\text{Keq\_PGI}} \cdot \frac{[\text{F6P}]}{\text{kmG6P\_PGI}}}{1 + \frac{[\text{G6P}]}{\text{kmG6P\_PGI}} + \frac{[\text{F6P}]}{\text{kmF6P\_PGI}}} \end{aligned} \tag{35}$$

Table 20: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Keq_PGI	Keq_PGI		0.430		☑
Vmax_PGI	Vmax_PGI		21.681		☑
kmF6P_PGI	kmF6P_PGI		3.139		☑
kmG6P_PGI	kmG6P_PGI		0.199		☑

6.5 Reaction re16

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

Name PFK

Reaction equation

$$\mathrm{F6P} + \mathrm{ATP} \xrightarrow{\mathrm{ADP,\ ATP,\ F6P,\ FBP}} \mathrm{FBP} + \mathrm{ADP} \tag{36}$$

Reactants

Table 21: Properties of each reactant.

Id	Name	SBO
F6P	F6P	
ATP	ATP	

Modifiers

Table 22: Properties of each modifier.

Id	Name	SBO
ADP	ADP	
ATP	ATP	
F6P	F6P	
FBP	FBP	

Products

Table 23: Properties of each product.

Id	Name	SBO
FBP	FBP	
ADP	ADP	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \mathrm{vol}\left(\mathrm{compartment\_1}\right) \cdot \mathrm{function\_4\_PFK}\left([\mathrm{ADP}], [\mathrm{ATP}], [\mathrm{F6P}], [\mathrm{FBP}], \mathrm{Vmax\_PFK}, \mathrm{kmADP\_PFK}, \mathrm{kmATP\_PFK}, \mathrm{kmF6P\_PFK}, \mathrm{kmFBP\_PFK}\right) \tag{37}$$

$$\begin{aligned}&\mathrm{function\_4\_PFK}\left([\mathrm{ADP}], [\mathrm{ATP}], [\mathrm{F6P}], [\mathrm{FBP}], \mathrm{Vmax\_PFK}, \mathrm{kmADP\_PFK}, \mathrm{kmATP\_PFK}, \mathrm{kmF6P\_PFK}, \mathrm{kmFBP\_PFK}\right) \\ &= \frac{\mathrm{Vmax\_PFK} \cdot \frac{[\mathrm{F6P}]}{\mathrm{kmF6P\_PFK}} \cdot \frac{[\mathrm{ATP}]}{\mathrm{kmATP\_PFK}}}{\left(1 + \frac{[\mathrm{F6P}]}{\mathrm{kmF6P\_PFK}}\right) \cdot \left(1 + \frac{[\mathrm{ATP}]}{\mathrm{kmATP\_PFK}}\right) + \left(1 + \frac{[\mathrm{FBP}]}{\mathrm{kmFBP\_PFK}}\right) \cdot \left(1 + \frac{[\mathrm{ADP}]}{\mathrm{kmADP\_PFK}}\right) - 1}\end{aligned} \tag{38}$$

$$\begin{aligned}&\mathrm{function\_4\_PFK}\left([\mathrm{ADP}], [\mathrm{ATP}], [\mathrm{F6P}], [\mathrm{FBP}], \mathrm{Vmax\_PFK}, \mathrm{kmADP\_PFK}, \mathrm{kmATP\_PFK}, \mathrm{kmF6P\_PFK}, \mathrm{kmFBP\_PFK}\right) \\ &= \frac{\mathrm{Vmax\_PFK} \cdot \frac{[\mathrm{F6P}]}{\mathrm{kmF6P\_PFK}} \cdot \frac{[\mathrm{ATP}]}{\mathrm{kmATP\_PFK}}}{\left(1 + \frac{[\mathrm{F6P}]}{\mathrm{kmF6P\_PFK}}\right) \cdot \left(1 + \frac{[\mathrm{ATP}]}{\mathrm{kmATP\_PFK}}\right) + \left(1 + \frac{[\mathrm{FBP}]}{\mathrm{kmFBP\_PFK}}\right) \cdot \left(1 + \frac{[\mathrm{ADP}]}{\mathrm{kmADP\_PFK}}\right) - 1}\end{aligned} \tag{39}$$

Table 24: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax_PFK	Vmax_PFK		18.358		☑
kmADP_PFK	kmADP_PFK		10.736		☑
kmATP_PFK	kmATP_PFK		0.062		☑
kmF6P_PFK	kmF6P_PFK		1.020		☑
kmFBP_PFK	kmFBP_PFK		86.805		☑

6.6 Reaction re17

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

Name FBA

Reaction equation

$$\mathrm{FBP} \xrightleftharpoons{\mathrm{FBP},\ \mathrm{G3P}} 2\,\mathrm{G3P} \tag{40}$$

Reactant

Table 25: Properties of each reactant.

Id	Name	SBO
FBP	FBP	

Modifiers

Table 26: Properties of each modifier.

Id	Name	SBO
FBP	FBP	
G3P	G3P	

Product

Table 27: Properties of each product.

Id	Name	SBO
G3P	G3P	

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \mathrm{vol}\left(\mathrm{compartment\_1}\right) \cdot \mathrm{function\_4\_FBA}\left([\mathrm{FBP}], [\mathrm{G3P}], \mathrm{Keq\_FBA}, \mathrm{Vmax\_FBA}, \mathrm{kmFBP\_FBA}, \mathrm{kmG3P\_FBA}\right) \tag{41}$$

$$\begin{aligned}&\mathrm{function\_4\_FBA}\left([\mathrm{FBP}], [\mathrm{G3P}], \mathrm{Keq\_FBA}, \mathrm{Vmax\_FBA}, \mathrm{kmFBP\_FBA}, \mathrm{kmG3P\_FBA}\right)\\ &= \frac{\mathrm{Vmax\_FBA} \cdot \frac{[\mathrm{FBP}]}{\mathrm{kmFBP\_FBA}} - \frac{\mathrm{Vmax\_FBA}}{\mathrm{Keq\_FBA}} \cdot \frac{[\mathrm{G3P}]^2}{\mathrm{kmFBP\_FBA}}}{1 + \frac{[\mathrm{FBP}]}{\mathrm{kmFBP\_FBA}} + \frac{[\mathrm{G3P}]}{\mathrm{kmG3P\_FBA}} + \left(\frac{[\mathrm{G3P}]}{\mathrm{kmG3P\_FBA}}\right)^2}\end{aligned} \tag{42}$$

$$\begin{aligned}&\text{function\_4\_FBA}\left([\text{FBP}], [\text{G3P}], \text{Keq\_FBA}, \text{Vmax\_FBA}, \text{kmFBP\_FBA}, \text{kmG3P\_FBA}\right)\\&= \frac{\text{Vmax\_FBA} \cdot \frac{[\text{FBP}]}{\text{kmFBP\_FBA}} - \frac{\text{Vmax\_FBA}}{\text{Keq\_FBA}} \cdot \frac{[\text{G3P}]^2}{\text{kmFBP\_FBA}}}{1 + \frac{[\text{FBP}]}{\text{kmFBP\_FBA}} + \frac{[\text{G3P}]}{\text{kmG3P\_FBA}} + \left(\frac{[\text{G3P}]}{\text{kmG3P\_FBA}}\right)^2}\end{aligned} \tag{43}$$

Table 28: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Keq_FBA	Keq_FBA		0.056		☑
Vmax_FBA	Vmax_FBA		56.131		☑
kmFBP_FBA	kmFBP_FBA		0.301		☑
kmG3P_FBA	kmG3P_FBA		10.106		☑

6.7 Reaction re18

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

Name GAPDH

Reaction equation

$$\text{G3P} + \text{Pint} + \text{NAD} \underset{\text{BPG, G3P, NAD, NADH, Pint}}{\rightleftharpoons} \text{BPG} + \text{NADH} \tag{44}$$

Reactants

Table 29: Properties of each reactant.

Id	Name	SBO
G3P	G3P	
Pint	Pint	
NAD	NAD	

Modifiers

Table 30: Properties of each modifier.

Id	Name	SBO
BPG	BPG	
G3P	G3P	
NAD	NAD	

Id	Name	SBO
NADH	NADH	
Pint	Pint	

Products

Table 31: Properties of each product.

Id	Name	SBO
BPG	BPG	
NADH	NADH	

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \mathrm{vol}\,(\mathrm{compartment\_1}) \cdot \mathrm{function\_4\_GAPDH}\,([\mathrm{BPG}], [\mathrm{G3P}], \mathrm{Keq\_GAPDH}, [\mathrm{NAD}], [\mathrm{NADH}], [\mathrm{Pint}], \mathrm{Vmax\_GAPDH}, \mathrm{kmBPG\_GAPDH}, \mathrm{kmG3P\_GAPDH}, \mathrm{kmNADH\_GAPDH}, \mathrm{kmNAD\_GAPDH}, \mathrm{kmPint\_GAPDH}) \tag{45}$$

$$\mathrm{function\_4\_GAPDH}\,([\mathrm{BPG}], [\mathrm{G3P}], \mathrm{Keq\_GAPDH}, [\mathrm{NAD}], [\mathrm{NADH}], [\mathrm{Pint}], \mathrm{Vmax\_GAPDH}, \mathrm{kmBPG\_GAPDH}, \mathrm{kmG3P\_GAPDH}, \mathrm{kmNADH\_GAPDH}, \mathrm{kmNAD\_GAPDH}, \mathrm{kmPint\_GAPDH}) = \frac{\mathrm{Vmax\_GAPDH} \cdot \frac{[\mathrm{G3P}]}{\mathrm{kmG3P\_GAPDH}} \cdot \frac{[\mathrm{NAD}]}{\mathrm{kmNAD\_GAPDH}} \cdot \frac{[\mathrm{Pint}]}{\mathrm{kmPint\_GAPDH}} - \frac{\mathrm{Vmax\_GAPDH}}{\mathrm{Keq\_GAPDH}}}{\left(1 + \frac{[\mathrm{G3P}]}{\mathrm{kmG3P\_GAPDH}}\right) \cdot \left(1 + \frac{[\mathrm{Pint}]}{\mathrm{kmPint\_GAPDH}}\right) \cdot \left(1 + \frac{[\mathrm{NAD}]}{\mathrm{kmNAD\_GAPDH}}\right) + \left(1 + \right.} \tag{46}$$

$$\mathrm{function\_4\_GAPDH}\,([\mathrm{BPG}], [\mathrm{G3P}], \mathrm{Keq\_GAPDH}, [\mathrm{NAD}], [\mathrm{NADH}], [\mathrm{Pint}], \mathrm{Vmax\_GAPDH}, \mathrm{kmBPG\_GAPDH}, \mathrm{kmG3P\_GAPDH}, \mathrm{kmNADH\_GAPDH}, \mathrm{kmNAD\_GAPDH}, \mathrm{kmPint\_GAPDH}) = \frac{\mathrm{Vmax\_GAPDH} \cdot \frac{[\mathrm{G3P}]}{\mathrm{kmG3P\_GAPDH}} \cdot \frac{[\mathrm{NAD}]}{\mathrm{kmNAD\_GAPDH}} \cdot \frac{[\mathrm{Pint}]}{\mathrm{kmPint\_GAPDH}} - \frac{\mathrm{Vmax\_GAPDH}}{\mathrm{Keq\_GAPDH}}}{\left(1 + \frac{[\mathrm{G3P}]}{\mathrm{kmG3P\_GAPDH}}\right) \cdot \left(1 + \frac{[\mathrm{Pint}]}{\mathrm{kmPint\_GAPDH}}\right) \cdot \left(1 + \frac{[\mathrm{NAD}]}{\mathrm{kmNAD\_GAPDH}}\right) + \left(1 + \right.} \tag{47}$$

Table 32: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Keq_GAPDH	Keq_GAPDH		$7 \cdot 10^{-4}$		☑
Vmax_GAPDH	Vmax_GAPDH		30.006		☑
kmBPG_GAPDH	kmBPG_GAPDH		0.048		☑
kmG3P_GAPDH	kmG3P_GAPDH		0.182		☑

Id	Name	SBO	Value	Unit	Constant
kmNADH_GAPDH	kmNADH-_GAPDH		0.643		☑
kmNAD_GAPDH	kmNAD_GAPDH		0.048		☑
kmPint_GAPDH	kmPint_GAPDH		6.753		☑

6.8 Reaction re20

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

Name ENO

Reaction equation

$$\mathrm{BPG} + \mathrm{ADP} \xrightleftharpoons{\text{ADP, ATP, BPG, PEP}} \mathrm{PEP} + \mathrm{ATP} \tag{48}$$

Reactants

Table 33: Properties of each reactant.

Id	Name	SBO
BPG	BPG	
ADP	ADP	

Modifiers

Table 34: Properties of each modifier.

Id	Name	SBO
ADP	ADP	
ATP	ATP	
BPG	BPG	
PEP	PEP	

Products

Table 35: Properties of each product.

Id	Name	SBO
PEP	PEP	
ATP	ATP	

Id	Name	SBO

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \mathrm{vol}(\mathrm{compartment\_1}) \cdot \mathrm{function\_4\_ENO}([\mathrm{ADP}], [\mathrm{ATP}], [\mathrm{BPG}], \mathrm{Keq\_ENO}, [\mathrm{PEP}], \mathrm{Vmax\_ENO}, \mathrm{kmADP\_ENO}, \mathrm{kmATP\_ENO}, \mathrm{kmBPG\_ENO}, \mathrm{kmPEP\_ENO}) \quad (49)$$

$$\mathrm{function\_4\_ENO}([\mathrm{ADP}], [\mathrm{ATP}], [\mathrm{BPG}], \mathrm{Keq\_ENO}, [\mathrm{PEP}], \mathrm{Vmax\_ENO}, \mathrm{kmADP\_ENO}, \mathrm{kmATP\_ENO}, \mathrm{kmBPG\_ENO}, \mathrm{kmPEP\_ENO}) = \frac{\mathrm{Vmax\_ENO} \cdot \frac{[\mathrm{BPG}]}{\mathrm{kmBPG\_ENO}} \cdot \frac{[\mathrm{ADP}]}{\mathrm{kmADP\_ENO}} - \frac{\mathrm{Vmax\_ENO}}{\mathrm{Keq\_ENO}} \cdot \frac{[\mathrm{PEP}]}{\mathrm{kmBPG\_ENO}} \cdot \frac{[\mathrm{ATP}]}{\mathrm{kmADP\_ENO}}}{\left(1 + \frac{[\mathrm{BPG}]}{\mathrm{kmBPG\_ENO}}\right) \cdot \left(1 + \frac{[\mathrm{ADP}]}{\mathrm{kmADP\_ENO}}\right) + \left(1 + \frac{[\mathrm{PEP}]}{\mathrm{kmPEP\_ENO}}\right) \cdot \left(1 + \frac{[\mathrm{ATP}]}{\mathrm{kmATP\_ENO}}\right) - 1} \quad (50)$$

$$\mathrm{function\_4\_ENO}([\mathrm{ADP}], [\mathrm{ATP}], [\mathrm{BPG}], \mathrm{Keq\_ENO}, [\mathrm{PEP}], \mathrm{Vmax\_ENO}, \mathrm{kmADP\_ENO}, \mathrm{kmATP\_ENO}, \mathrm{kmBPG\_ENO}, \mathrm{kmPEP\_ENO}) = \frac{\mathrm{Vmax\_ENO} \cdot \frac{[\mathrm{BPG}]}{\mathrm{kmBPG\_ENO}} \cdot \frac{[\mathrm{ADP}]}{\mathrm{kmADP\_ENO}} - \frac{\mathrm{Vmax\_ENO}}{\mathrm{Keq\_ENO}} \cdot \frac{[\mathrm{PEP}]}{\mathrm{kmBPG\_ENO}} \cdot \frac{[\mathrm{ATP}]}{\mathrm{kmADP\_ENO}}}{\left(1 + \frac{[\mathrm{BPG}]}{\mathrm{kmBPG\_ENO}}\right) \cdot \left(1 + \frac{[\mathrm{ADP}]}{\mathrm{kmADP\_ENO}}\right) + \left(1 + \frac{[\mathrm{PEP}]}{\mathrm{kmPEP\_ENO}}\right) \cdot \left(1 + \frac{[\mathrm{ATP}]}{\mathrm{kmATP\_ENO}}\right) - 1} \quad (51)$$

Table 36: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
`Keq_ENO`	Keq_ENO		27.550		☑
`Vmax_ENO`	Vmax_ENO		29.132		☑
`kmADP_ENO`	kmADP_ENO		0.413		☑
`kmATP_ENO`	kmATP_ENO		0.748		☑
`kmBPG_ENO`	kmBPG_ENO		0.024		☑
`kmPEP_ENO`	kmPEP_ENO		1.389		☑

6.9 Reaction `re21`

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

Name PYK

Reaction equation

$$\mathrm{PEP} + \mathrm{ADP} \xrightarrow{\mathrm{FBP,\ Pint,\ ADP,\ ATP,\ FBP,\ PEP,\ PYR,\ Pint}} \mathrm{PYR} + \mathrm{ATP} \tag{52}$$

Reactants

Table 37: Properties of each reactant.

Id	Name	SBO
PEP	PEP	
ADP	ADP	

Modifiers

Table 38: Properties of each modifier.

Id	Name	SBO
FBP	FBP	
Pint	Pint	
ADP	ADP	
ATP	ATP	
FBP	FBP	
PEP	PEP	
PYR	PYR	
Pint	Pint	

Products

Table 39: Properties of each product.

Id	Name	SBO
PYR	PYR	
ATP	ATP	

Kinetic Law

Derived unit contains undeclared units

$$\begin{aligned} v_9 = {} & \mathrm{vol}(\mathrm{compartment\_1}) \\ & \cdot \mathrm{function\_4\_PYK}([\mathrm{ADP}], [\mathrm{ATP}], [\mathrm{FBP}], [\mathrm{PEP}], [\mathrm{PYR}], [\mathrm{Pint}], \mathrm{Vmax\_PYK}, \mathrm{kaFBP\_PYK}, \\ & \quad \mathrm{kiPint\_PYK}, \mathrm{kmADP\_PYK}, \mathrm{kmATP\_PYK}, \mathrm{kmPEP\_PYK}, \mathrm{kmPYR\_PYK}, \mathrm{nPYK}) \end{aligned} \tag{53}$$

$$\text{function\_4\_PYK}([\text{ADP}], [\text{ATP}], [\text{FBP}], [\text{PEP}], [\text{PYR}], [\text{Pint}], \text{Vmax\_PYK}, \text{kaFBP\_PYK}, \text{kiPint\_PYK}, \text{kmADP\_PYK}, \text{kmATP\_PYK}, \text{kmPEP\_PYK}, \text{kmPYR\_PYK}, \text{nPYK}) = \frac{\frac{[\text{FBP}]}{[\text{FBP}]+\text{kaFBP\_PYK}} \cdot \frac{\text{kiPint\_PYK}^{\text{nPYK}}}{[\text{Pint}]^{\text{nPYK}}+\text{kiPint\_PYK}^{\text{nPYK}}} \cdot \text{Vmax\_PYK} \cdot \frac{[\text{ADP}]}{\text{kmADP\_PYK}} \cdot \frac{[\text{PEP}]}{\text{kmPEP\_PYK}}}{\left(1+\frac{[\text{ADP}]}{\text{kmADP\_PYK}}\right) \cdot \left(1+\frac{[\text{PEP}]}{\text{kmPEP\_PYK}}\right) + \left(1+\frac{[\text{ATP}]}{\text{kmATP\_PYK}}\right) \cdot \left(1+\frac{[\text{PYR}]}{\text{kmPYR\_PYK}}\right) - 1} \tag{54}$$

$$\text{function\_4\_PYK}([\text{ADP}], [\text{ATP}], [\text{FBP}], [\text{PEP}], [\text{PYR}], [\text{Pint}], \text{Vmax\_PYK}, \text{kaFBP\_PYK}, \text{kiPint\_PYK}, \text{kmADP\_PYK}, \text{kmATP\_PYK}, \text{kmPEP\_PYK}, \text{kmPYR\_PYK}, \text{nPYK}) = \frac{\frac{[\text{FBP}]}{[\text{FBP}]+\text{kaFBP\_PYK}} \cdot \frac{\text{kiPint\_PYK}^{\text{nPYK}}}{[\text{Pint}]^{\text{nPYK}}+\text{kiPint\_PYK}^{\text{nPYK}}} \cdot \text{Vmax\_PYK} \cdot \frac{[\text{ADP}]}{\text{kmADP\_PYK}} \cdot \frac{[\text{PEP}]}{\text{kmPEP\_PYK}}}{\left(1+\frac{[\text{ADP}]}{\text{kmADP\_PYK}}\right) \cdot \left(1+\frac{[\text{PEP}]}{\text{kmPEP\_PYK}}\right) + \left(1+\frac{[\text{ATP}]}{\text{kmATP\_PYK}}\right) \cdot \left(1+\frac{[\text{PYR}]}{\text{kmPYR\_PYK}}\right) - 1} \tag{55}$$

Table 40: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax_PYK	Vmax_PYK		2.224		☑
kaFBP_PYK	kaFBP_PYK		0.039		☑
kiPint_PYK	kiPint_PYK		3.701		☑
kmADP_PYK	kmADP_PYK		3.077		☑
kmATP_PYK	kmATP_PYK		29.603		☑
kmPEP_PYK	kmPEP_PYK		0.331		☑
kmPYR_PYK	kmPYR_PYK		96.423		☑
nPYK	nPYK		3.000		☑

6.10 Reaction re22

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

Name LDH

Reaction equation

$$\text{PYR} + \text{NADH} \xrightarrow{\text{FBP, Pint, FBP, Lactate, NAD, NADH, PYR, Pint}} \text{Lactate} + \text{NAD} \tag{56}$$

Reactants

Table 41: Properties of each reactant.

Id	Name	SBO
PYR	PYR	
NADH	NADH	

Modifiers

Table 42: Properties of each modifier.

Id	Name	SBO
FBP	FBP	
Pint	Pint	
FBP	FBP	
Lactate	Lactate	
NAD	NAD	
NADH	NADH	
PYR	PYR	
Pint	Pint	

Products

Table 43: Properties of each product.

Id	Name	SBO
Lactate	Lactate	
NAD	NAD	

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = \text{function\_4\_LDH}([\text{FBP}], [\text{Lactate}], [\text{NAD}], [\text{NADH}], [\text{PYR}], [\text{Pint}], \text{Vmax\_LDH}, \text{kaFBP\_LDH}, \text{kiPint\_LDH}, \text{kmLactate\_LDH}, \text{kmNADH\_LDH}, \text{kmNAD\_LDH}, \text{kmPYR\_LDH}) \quad (57)$$

$$\text{function\_4\_LDH}([\text{FBP}], [\text{Lactate}], [\text{NAD}], [\text{NADH}], [\text{PYR}], [\text{Pint}], \text{Vmax\_LDH}, \text{kaFBP\_LDH}, \text{kiPint\_LDH}, \text{kmLactate\_LDH}, \text{kmNADH\_LDH}, \text{kmNAD\_LDH}, \text{kmPYR\_LDH}) = \frac{\frac{[\text{FBP}]}{[\text{FBP}]+\text{kaFBP\_LDH}} \cdot \frac{\text{kiPint\_LDH}}{[\text{Pint}]+\text{kiPint\_LDH}} \cdot \text{Vmax\_LDH} \cdot \frac{[\text{PYR}]}{\text{kmPYR\_LDH}} \cdot \frac{[\text{NADH}]}{\text{kmNADH\_LDH}}}{\left(1 + \frac{[\text{PYR}]}{\text{kmPYR\_LDH}}\right) \cdot \left(1 + \frac{[\text{NADH}]}{\text{kmNADH\_LDH}}\right) + \left(1 + \frac{[\text{Lactate}]}{\text{kmLactate\_LDH}}\right) \cdot \left(1 + \frac{[\text{NAD}]}{\text{kmNAD\_LDH}}\right) - 1} \quad (58)$$

Table 44: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax_LDH	Vmax_LDH		566.598		☑
kaFBP_LDH	kaFBP_LDH		0.018		☑
kiPint_LDH	kiPint_LDH		0.068		☑
kmLactate-_LDH	kmLactate_LDH		94.120		☑
kmNADH_LDH	kmNADH_LDH		0.144		☑
kmNAD_LDH	kmNAD_LDH		3.084		☑
kmPYR_LDH	kmPYR_LDH		0.010		☑

6.11 Reaction re23

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

Name PDH

Reaction equation

$$\mathrm{PYR} + \mathrm{CoA} \xrightleftharpoons{\text{G3P, AcetCoA, CoA, Formate, G3P, PYR}} \mathrm{AcetCoA} + \mathrm{Formate} \qquad (59)$$

Reactants

Table 45: Properties of each reactant.

Id	Name	SBO
PYR	PYR	
CoA	CoA	

Modifiers

Table 46: Properties of each modifier.

Id	Name	SBO
G3P	G3P	
AcetCoA	AcetCoA	
CoA	CoA	
Formate	Formate	
G3P	G3P	
PYR	PYR	

Products

Table 47: Properties of each product.

Id	Name	SBO
AcetCoA	AcetCoA	
Formate	Formate	

Kinetic Law

Derived unit contains undeclared units

$$v_{11} = \text{function\_4\_PFL}([\text{AcetCoA}], [\text{CoA}], [\text{Formate}], [\text{G3P}], \text{Keq\_PFL}, \text{KmCoA\_PFL}, [\text{PYR}], \text{Vmax\_PFL}, \text{kiG3P\_PFL}, \text{kmAcetCoA\_PFL}, \text{kmFormate\_PFL}, \text{kmPYR\_PFL}) \tag{60}$$

$$\begin{aligned}&\text{function\_4\_PFL}([\text{AcetCoA}], [\text{CoA}], [\text{Formate}], [\text{G3P}], \text{Keq\_PFL}, \text{KmCoA\_PFL}, \\ &[\text{PYR}], \text{Vmax\_PFL}, \text{kiG3P\_PFL}, \text{kmAcetCoA\_PFL}, \text{kmFormate\_PFL}, \text{kmPYR\_PFL}) \\ &= \frac{\frac{\text{kiG3P\_PFL}}{[\text{G3P}]+\text{kiG3P\_PFL}} \cdot \left(\text{Vmax\_PFL} \cdot \frac{[\text{PYR}]}{\text{kmPYR\_PFL}} \cdot \frac{[\text{CoA}]}{\text{KmCoA\_PFL}} - \frac{\text{Vmax\_PFL}}{\text{Keq\_PFL}} \cdot \frac{[\text{AcetCoA}]}{\text{kmPYR\_PFL}} \cdot \frac{[\text{Formate}]}{\text{KmCoA\_PFL}}\right)}{\left(1 + \frac{[\text{PYR}]}{\text{kmPYR\_PFL}}\right) \cdot \left(1 + \frac{[\text{CoA}]}{\text{KmCoA\_PFL}}\right) + \left(1 + \frac{[\text{AcetCoA}]}{\text{kmAcetCoA\_PFL}}\right) \cdot \left(1 + \frac{[\text{Formate}]}{\text{kmFormate\_PFL}}\right) - 1}\end{aligned} \tag{61}$$

Table 48: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Keq_PFL	Keq_PFL		650.000		☑
KmCoA_PFL	KmCoA_PFL		0.124		☑
Vmax_PFL	Vmax_PFL		0.002		☑
kiG3P_PFL	kiG3P_PFL		0.511		☑
kmAcetCoA_PFL	kmAcetCoA_PFL		7.343		☑
kmFormate_PFL	kmFormate_PFL		54.269		☑
kmPYR_PFL	kmPYR_PFL		5.777		☑

6.12 Reaction re24

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

Name AE

Reaction equation

$$\mathrm{AcetCoA} + 2\,\mathrm{NADH} \xrightarrow{\mathrm{ATP,\ ATP,\ AcetCoA,\ CoA,\ Ethanol,\ NAD,\ NADH}} \mathrm{Ethanol} + 2\,\mathrm{NAD} + \mathrm{CoA} \tag{62}$$

Reactants

Table 49: Properties of each reactant.

Id	Name	SBO
AcetCoA	AcetCoA	
NADH	NADH	

Modifiers

Table 50: Properties of each modifier.

Id	Name	SBO
ATP	ATP	
ATP	ATP	
AcetCoA	AcetCoA	
CoA	CoA	
Ethanol	Ethanol	
NAD	NAD	
NADH	NADH	

Products

Table 51: Properties of each product.

Id	Name	SBO
Ethanol	Ethanol	
NAD	NAD	
CoA	CoA	

Kinetic Law

Derived unit contains undeclared units

$$v_{12} = \text{function\_4\_AE}([\text{ATP}], [\text{AcetCoA}], [\text{CoA}], [\text{Ethanol}], [\text{NAD}], [\text{NADH}], \text{Vmax\_AE}, \text{kiATP\_AE}, \text{kmAcetCoA\_AE}, \text{kmCoA\_AE}, \text{kmEthanol\_AE}, \text{kmNADH\_AE}, \text{kmNAD\_AE}) \tag{63}$$

$$\text{function\_4\_AE}([\text{ATP}], [\text{AcetCoA}], [\text{CoA}], [\text{Ethanol}], [\text{NAD}], [\text{NADH}], \text{Vmax\_AE}, \text{kiATP\_AE}, \text{kmAcetCoA\_AE}, \text{kmCoA\_AE}, \text{kmEthanol\_AE}, \text{kmNADH\_AE}, \text{kmNAD\_AE}) \tag{64}$$

$$= \frac{\frac{\text{kiATP\_AE}}{[\text{ATP}]+\text{kiATP\_AE}} \cdot \text{Vmax\_AE} \cdot \frac{[\text{AcetCoA}]}{\text{kmAcetCoA\_AE}} \cdot \left(\frac{[\text{NADH}]}{\text{kmNADH\_AE}}\right)^2}{\left(1 + \frac{[\text{NADH}]}{\text{kmNADH\_AE}} + \left(\frac{[\text{NADH}]}{\text{kmNADH\_AE}}\right)^2\right) \cdot \left(1 + \frac{[\text{AcetCoA}]}{\text{kmAcetCoA\_AE}}\right) + \left(1 + \frac{[\text{Ethanol}]}{\text{kmEthanol\_AE}}\right) \cdot \left(1 + \frac{[\text{CoA}]}{\text{kmCoA\_AE}}\right) \cdot \left(1 + \frac{[\text{NA}}{\text{kmNA}}\right.}$$

Table 52: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
`Vmax_AE`	Vmax_AE		2.118		☑
`kiATP_AE`	kiATP_AE		6.281		☑
`kmAcetCoA_AE`	kmAcetCoA_AE		7.380		☑
`kmCoA_AE`	kmCoA_AE		0.092		☑
`kmEthanol_AE`	kmEthanol_AE		2.281		☑
`kmNADH_AE`	kmNADH_AE		0.431		☑
`kmNAD_AE`	kmNAD_AE		1.314		☑

6.13 Reaction `re25`

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

Name AC

Reaction equation

$$\text{AcetCoA} + \text{ADP} \xrightarrow{\text{ADP, ATP, AcetCoA, Acetate, CoA}} \text{Acetate} + \text{ATP} + \text{CoA} \tag{65}$$

Reactants

Table 53: Properties of each reactant.

Id	Name	SBO
`AcetCoA`	AcetCoA	
`ADP`	ADP	

Modifiers

Table 54: Properties of each modifier.

Id	Name	SBO
ADP	ADP	
ATP	ATP	
AcetCoA	AcetCoA	
Acetate	Acetate	
CoA	CoA	

Products

Table 55: Properties of each product.

Id	Name	SBO
Acetate	Acetate	
ATP	ATP	
CoA	CoA	

Kinetic Law

Derived unit contains undeclared units

$$v_{13} = \text{function\_4\_ACK}([\text{ADP}], [\text{ATP}], [\text{AcetCoA}], [\text{Acetate}], [\text{CoA}], \text{Vmax\_ACK}, \text{kmADP\_ACK}, \text{kmATP\_ACK}, \text{kmAcetCoA\_ACK}, \text{kmAcetate\_ACK}, \text{kmCoA\_ACK}) \tag{66}$$

$$\text{function\_4\_ACK}([\text{ADP}], [\text{ATP}], [\text{AcetCoA}], [\text{Acetate}], [\text{CoA}], \text{Vmax\_ACK}, \text{kmADP\_ACK}, \text{kmATP\_ACK}, \text{kmAcetCoA\_ACK}, \text{kmAcetate\_ACK}, \text{kmCoA\_ACK}) \tag{67}$$

$$= \frac{\text{Vmax\_ACK} \cdot \frac{[\text{AcetCoA}]}{\text{kmAcetCoA\_ACK}} \cdot \frac{[\text{ADP}]}{\text{kmADP\_ACK}}}{\left(1 + \frac{[\text{AcetCoA}]}{\text{kmAcetCoA\_ACK}}\right) \cdot \left(1 + \frac{[\text{ADP}]}{\text{kmADP\_ACK}}\right) + \left(1 + \frac{[\text{Acetate}]}{\text{kmAcetate\_ACK}}\right) \cdot \left(1 + \frac{[\text{ATP}]}{\text{kmATP\_ACK}}\right) \cdot \left(1 + \frac{[\text{CoA}]}{\text{kmCoA\_ACK}}\right) - 1}$$

Table 56: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax_ACK	Vmax_ACK		3.839		☑
kmADP_ACK	kmADP_ACK		1.172		☑
kmATP_ACK	kmATP_ACK		14.156		☑

Id	Name	SBO	Value	Unit	Constant
kmAcetCoA-_ACK	kmAcetCoA_ACK		0.558		☑
kmAcetate-_ACK	kmAcetate_ACK		0.552		☑
kmCoA_ACK	kmCoA_ACK		0.173		☑

6.14 Reaction re26

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

Name PA

Reaction equation

$$2\,\mathrm{PYR} \overset{\text{Acetoin, PYR}}{\rightleftharpoons} \text{Acetoin} \tag{68}$$

Reactant

Table 57: Properties of each reactant.

Id	Name	SBO
PYR	PYR	

Modifiers

Table 58: Properties of each modifier.

Id	Name	SBO
Acetoin	Acetoin	
PYR	PYR	

Product

Table 59: Properties of each product.

Id	Name	SBO
Acetoin	Acetoin	

Kinetic Law

Derived unit contains undeclared units

$$v_{14} = \mathrm{vol}\left(\mathrm{compartment\_1}\right) \cdot \mathrm{function\_4\_ALS}\left([\mathrm{Acetoin}], \mathrm{Keq\_ALS}, [\mathrm{PYR}], \mathrm{Vmax\_ALS}, \mathrm{kmAcetoin\_ALS}, \mathrm{kmPYR\_ALS}\right) \tag{69}$$

$$\mathrm{function\_4\_ALS}\left([\mathrm{Acetoin}], \mathrm{Keq\_ALS}, [\mathrm{PYR}], \mathrm{Vmax\_ALS}, \mathrm{kmAcetoin\_ALS}, \mathrm{kmPYR\_ALS}\right) = \frac{\mathrm{Vmax\_ALS} \cdot \left(\frac{[\mathrm{PYR}]}{\mathrm{kmPYR\_ALS}}\right)^2 - \frac{\mathrm{Vmax\_ALS}}{\mathrm{Keq\_ALS}} \cdot \frac{[\mathrm{Acetoin}]}{\mathrm{kmPYR\_ALS}}}{1 + \frac{[\mathrm{PYR}]}{\mathrm{kmPYR\_ALS}} + \left(\frac{[\mathrm{PYR}]}{\mathrm{kmPYR\_ALS}}\right)^2 + 1 + \frac{[\mathrm{Acetoin}]}{\mathrm{kmAcetoin\_ALS}} - 1} \tag{70}$$

$$\mathrm{function\_4\_ALS}\left([\mathrm{Acetoin}], \mathrm{Keq\_ALS}, [\mathrm{PYR}], \mathrm{Vmax\_ALS}, \mathrm{kmAcetoin\_ALS}, \mathrm{kmPYR\_ALS}\right) = \frac{\mathrm{Vmax\_ALS} \cdot \left(\frac{[\mathrm{PYR}]}{\mathrm{kmPYR\_ALS}}\right)^2 - \frac{\mathrm{Vmax\_ALS}}{\mathrm{Keq\_ALS}} \cdot \frac{[\mathrm{Acetoin}]}{\mathrm{kmPYR\_ALS}}}{1 + \frac{[\mathrm{PYR}]}{\mathrm{kmPYR\_ALS}} + \left(\frac{[\mathrm{PYR}]}{\mathrm{kmPYR\_ALS}}\right)^2 + 1 + \frac{[\mathrm{Acetoin}]}{\mathrm{kmAcetoin\_ALS}} - 1} \tag{71}$$

Table 60: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
`Keq_ALS`	Keq_ALS		900000.000		☑
`Vmax_ALS`	Vmax_ALS		0.355		☑
`kmAcetoin_ALS`	kmAcetoin_ALS		0.050		☑
`kmPYR_ALS`	kmPYR_ALS		0.263		☑

6.15 Reaction `re27`

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

Name AB

Reaction equation

$$\mathrm{Acetoin} + \mathrm{NADH} \xrightleftharpoons{\text{Acetoin, Butanediol, NAD, NADH}} \mathrm{Butanediol} + \mathrm{NAD} \tag{72}$$

Reactants

Table 61: Properties of each reactant.

Id	Name	SBO
Acetoin	Acetoin	
NADH	NADH	

Modifiers

Table 62: Properties of each modifier.

Id	Name	SBO
Acetoin	Acetoin	
Butanediol	Butanediol	
NAD	NAD	
NADH	NADH	

Products

Table 63: Properties of each product.

Id	Name	SBO
Butanediol	Butanediol	
NAD	NAD	

Kinetic Law

Derived unit contains undeclared units

$$v_{15} = \text{function\_4\_BDH}\left([\text{Acetoin}], [\text{Butanediol}], \text{Keq\_BDH}, [\text{NAD}], [\text{NADH}], \text{Vmax\_BDH}, \text{kmAcetoin\_BDH}, \text{kmButanediol\_BDH}, \text{kmNADH\_BDH}, \text{kmNAD\_BDH}\right) \tag{73}$$

$$\begin{aligned}&\text{function\_4\_BDH}\left([\text{Acetoin}], [\text{Butanediol}], \text{Keq\_BDH}, [\text{NAD}], [\text{NADH}], \text{Vmax\_BDH}, \text{kmAcetoin\_BDH}, \text{kmButanediol\_BDH}, \text{kmNADH\_BDH}, \text{kmNAD\_BDH}\right)\\ &= \frac{\text{Vmax\_BDH} \cdot \frac{[\text{Acetoin}]}{\text{kmAcetoin\_BDH}} \cdot \frac{[\text{NADH}]}{\text{kmNADH\_BDH}} - \frac{\text{Vmax\_BDH}}{\text{Keq\_BDH}} \cdot \frac{[\text{Butanediol}]}{\text{kmAcetoin\_BDH}} \cdot \frac{[\text{NAD}]}{\text{kmNADH\_BDH}}}{\left(1 + \frac{[\text{Acetoin}]}{\text{kmAcetoin\_BDH}}\right) \cdot \left(1 + \frac{[\text{NADH}]}{\text{kmNADH\_BDH}}\right) + \left(1 + \frac{[\text{Butanediol}]}{\text{kmButanediol\_BDH}}\right) \cdot \left(1 + \frac{[\text{NAD}]}{\text{kmNAD\_BDH}}\right) - 1}\end{aligned} \tag{74}$$

Table 64: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Keq_BDH	Keq_BDH		1400.000		☑
Vmax_BDH	Vmax_BDH		2.286		☑
kmAcetoin-_BDH	kmAcetoin_BDH		5.624		☑
kmButanediol-_BDH	kmButanediol-_BDH		1.807		☑
kmNADH_BDH	kmNADH_BDH		3.549		☑
kmNAD_BDH	kmNAD_BDH		1.296		☑

6.16 Reaction re28

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

Name MPD

Reaction equation

$$\mathrm{F6P} + \mathrm{NADH} \xrightleftharpoons{\text{F6P, F6P, Mannitol1Phosphate, NAD, NADH}} \mathrm{Mannitol1Phosphate} + \mathrm{NAD} \tag{75}$$

Reactants

Table 65: Properties of each reactant.

Id	Name	SBO
F6P	F6P	
NADH	NADH	

Modifiers

Table 66: Properties of each modifier.

Id	Name	SBO
F6P	F6P	
F6P	F6P	
Mannitol1Phosphate	Mannitol1Phosphate	
NAD	NAD	
NADH	NADH	

Products

Table 67: Properties of each product.

Id	Name	SBO
Mannitol1Phosphate	Mannitol1Phosphate	
NAD	NAD	

Kinetic Law

Derived unit contains undeclared units

$$v_{16} = \mathrm{vol}(\mathrm{compartment\_1}) \cdot \mathrm{function\_4\_MPD}([\mathrm{F6P}], \mathrm{Keq\_MPD}, [\mathrm{Mannitol1Phosphate}], [\mathrm{NAD}], [\mathrm{NADH}], \mathrm{Vmax\_MPD}, \mathrm{kiF6P\_MPD}, \mathrm{kmF6P\_MPD}, \mathrm{kmMannitol1Phoshate\_MPD}, \mathrm{kmNADH\_MPD}, \mathrm{kmNAD\_MPD}) \tag{76}$$

$$\mathrm{function\_4\_MPD}([\mathrm{F6P}], \mathrm{Keq\_MPD}, [\mathrm{Mannitol1Phosphate}], [\mathrm{NAD}], [\mathrm{NADH}], \mathrm{Vmax\_MPD}, \mathrm{kiF6P\_MPD}, \mathrm{kmF6P\_MPD}, \mathrm{kmMannitol1Phoshate\_MPD}, \mathrm{kmNADH\_MPD}, \mathrm{kmNAD\_MPD}) = \frac{\frac{\mathrm{kiF6P\_MPD}}{[\mathrm{F6P}]+\mathrm{kiF6P\_MPD}} \cdot \left(\mathrm{Vmax\_MPD} \cdot \frac{[\mathrm{F6P}]}{\mathrm{kmF6P\_MPD}} \cdot \frac{[\mathrm{NADH}]}{\mathrm{kmNADH\_MPD}} - \frac{\mathrm{Vmax\_MPD}}{\mathrm{Keq\_MPD}} \cdot \frac{[\mathrm{Mannitol1Phosphate}]}{\mathrm{kmF6P\_MPD}} \cdot \frac{[\mathrm{NA}}{\mathrm{kmNADH}}\right.}{\left(1 + \frac{[\mathrm{F6P}]}{\mathrm{kmF6P\_MPD}}\right) \cdot \left(1 + \frac{[\mathrm{NADH}]}{\mathrm{kmNADH\_MPD}}\right) + \left(1 + \frac{[\mathrm{Mannitol1Phosphate}]}{\mathrm{kmMannitol1Phoshate\_MPD}}\right) \cdot \left(1 + \frac{[\mathrm{NAD}]}{\mathrm{kmNAD\_MPD}}\right) - \left.\right.} \tag{77}$$

$$\mathrm{function\_4\_MPD}([\mathrm{F6P}], \mathrm{Keq\_MPD}, [\mathrm{Mannitol1Phosphate}], [\mathrm{NAD}], [\mathrm{NADH}], \mathrm{Vmax\_MPD}, \mathrm{kiF6P\_MPD}, \mathrm{kmF6P\_MPD}, \mathrm{kmMannitol1Phoshate\_MPD}, \mathrm{kmNADH\_MPD}, \mathrm{kmNAD\_MPD}) = \frac{\frac{\mathrm{kiF6P\_MPD}}{[\mathrm{F6P}]+\mathrm{kiF6P\_MPD}} \cdot \left(\mathrm{Vmax\_MPD} \cdot \frac{[\mathrm{F6P}]}{\mathrm{kmF6P\_MPD}} \cdot \frac{[\mathrm{NADH}]}{\mathrm{kmNADH\_MPD}} - \frac{\mathrm{Vmax\_MPD}}{\mathrm{Keq\_MPD}} \cdot \frac{[\mathrm{Mannitol1Phosphate}]}{\mathrm{kmF6P\_MPD}} \cdot \frac{[\mathrm{NA}}{\mathrm{kmNADH}}\right.}{\left(1 + \frac{[\mathrm{F6P}]}{\mathrm{kmF6P\_MPD}}\right) \cdot \left(1 + \frac{[\mathrm{NADH}]}{\mathrm{kmNADH\_MPD}}\right) + \left(1 + \frac{[\mathrm{Mannitol1Phosphate}]}{\mathrm{kmMannitol1Phoshate\_MPD}}\right) \cdot \left(1 + \frac{[\mathrm{NAD}]}{\mathrm{kmNAD\_MPD}}\right) - \left.\right.} \tag{78}$$

Table 68: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Keq_MPD	Keq_MPD		200.000		☑
Vmax_MPD	Vmax_MPD		1.327		☑
kiF6P_MPD	kiF6P_MPD		22.028		☑
kmF6P_MPD	kmF6P_MPD		0.321		☑
kmMannitol1Phoshate_MPD	kmMannitol1Phoshate_MPD		0.089		☑
kmNADH_MPD	kmNADH_MPD		0.030		☑
kmNAD_MPD	kmNAD_MPD		0.373		☑

6.17 Reaction re29

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

Name MP

Reaction equation

$$\text{Mannitol1Phosphate} \xrightarrow{\text{Mannitol, Mannitol1Phosphate}} \text{Mannitol} \tag{79}$$

Reactant

Table 69: Properties of each reactant.

Id	Name	SBO
Mannitol1Phosphate	Mannitol1Phosphate	

Modifiers

Table 70: Properties of each modifier.

Id	Name	SBO
Mannitol	Mannitol	
Mannitol1Phosphate	Mannitol1Phosphate	

Product

Table 71: Properties of each product.

Id	Name	SBO
Mannitol	Mannitol	

Kinetic Law

Derived unit contains undeclared units

$$v_{17} = \text{vol}(\text{compartment\_1}) \cdot \text{function\_4\_MP}([\text{Mannitol}], [\text{Mannitol1Phosphate}], \text{Vmax\_MP}, \text{kmMannitol1Phosphate\_MP}, \text{kmMannitol\_MP}) \tag{80}$$

$$\text{function\_4\_MP}([\text{Mannitol}], [\text{Mannitol1Phosphate}], \text{Vmax\_MP}, \text{kmMannitol1Phosphate\_MP}, \text{kmMannitol\_MP}) = \frac{\text{Vmax\_MP} \cdot \frac{[\text{Mannitol1Phosphate}]}{\text{kmMannitol1Phosphate\_MP}}}{1 + \frac{[\text{Mannitol1Phosphate}]}{\text{kmMannitol1Phosphate\_MP}} + 1 + \frac{[\text{Mannitol}]}{\text{kmMannitol\_MP}} - 1} \tag{81}$$

$$\text{function\_4\_MP}([\text{Mannitol}], [\text{Mannitol1Phosphate}], \text{Vmax\_MP}, \text{kmMannitol1Phosphate\_MP}, \text{kmMannitol\_MP}) = \frac{\text{Vmax\_MP} \cdot \frac{[\text{Mannitol1Phosphate}]}{\text{kmMannitol1Phosphate\_MP}}}{1 + \frac{[\text{Mannitol1Phosphate}]}{\text{kmMannitol1Phosphate\_MP}} + 1 + \frac{[\text{Mannitol}]}{\text{kmMannitol\_MP}} - 1} \tag{82}$$

Table 72: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax_MP	Vmax_MP		3.486		☑
kmMannitol1Phosphate_MP	kmMannitol1Phosphate_MP		3.516		☑
kmMannitol_MP	kmMannitol_MP		0.239		☑

6.18 Reaction re30

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

Name PTS_Man

Reaction equation

$$\text{Mannitol\_Ext} + \text{PEP} \xrightarrow{\text{Mannitol1Phosphate, Mannitol\_Ext, PEP, PYR}} \text{Mannitol1Phosphate} + \text{PYR} \tag{83}$$

Reactants

Table 73: Properties of each reactant.

Id	Name	SBO
Mannitol_Ext	Mannitol_Ext	
PEP	PEP	

Modifiers

Table 74: Properties of each modifier.

Id	Name	SBO
Mannitol1Phosphate	Mannitol1Phosphate	
Mannitol_Ext	Mannitol_Ext	
PEP	PEP	
PYR	PYR	

Products

Table 75: Properties of each product.

Id	Name	SBO
Mannitol1Phosphate	Mannitol1Phosphate	
PYR	PYR	

Kinetic Law

Derived unit contains undeclared units

$$v_{18} = \text{function\_4\_PTS\_Man}([\text{Mannitol1Phosphate}], [\text{Mannitol\_Ext}], [\text{PEP}], [\text{PYR}], \text{Vmax\_PTS\_Man}, \text{kmMannitol1Phosphate\_PTS\_Man}, \text{kmMannitolExt\_PTS\_Man}, \text{kmPEP\_PTS\_Man}, \text{kmPYR\_PTS\_Man}) \quad (84)$$

$$\text{function\_4\_PTS\_Man}([\text{Mannitol1Phosphate}], [\text{Mannitol\_Ext}], [\text{PEP}], [\text{PYR}], \text{Vmax\_PTS\_Man}, \text{kmMannitol1Phosphate\_PTS\_Man}, \text{kmMannitolExt\_PTS\_Man}, \text{kmPEP\_PTS\_Man}, \text{kmPYR\_PTS\_Man}) \quad (85)$$

$$= \frac{\text{Vmax\_PTS\_Man} \cdot \frac{[\text{Mannitol\_Ext}]}{\text{kmMannitolExt\_PTS\_Man}} \cdot \frac{[\text{PEP}]}{\text{kmPEP\_PTS\_Man}}}{\left(1 + \frac{[\text{Mannitol\_Ext}]}{\text{kmMannitolExt\_PTS\_Man}}\right) \cdot \left(1 + \frac{[\text{PEP}]}{\text{kmPEP\_PTS\_Man}}\right) + \left(1 + \frac{[\text{Mannitol1Phosphate}]}{\text{kmMannitol1Phosphate\_PTS\_Man}}\right) \cdot \left(1 + \frac{[\text{PYR}]}{\text{kmPYR\_PTS\_Man}}\right) - 1}$$

Table 76: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax_PTS_Man	Vmax_PTS_Man		4.449		☑
kmMannitol1Phosphate-_PTS_Man	kmMannitol1Phosphate-_PTS_Man		0.363		☑
kmMannitolExt-_PTS_Man	kmMannitolExt-_PTS_Man		0.013		☑

Id	Name	SBO	Value	Unit	Constant
kmPEP_PTS-_Man	kmPEP_PTS_Man		2.208		☑
kmPYR_PTS-_Man	kmPYR_PTS_Man		0.344		☑

6.19 Reaction re31

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

Name Acetoin_transp

Reaction equation

$$\text{Acetoin} \xrightarrow{\text{Acetoin, Acetoin\_Ext}} \text{Acetoin\_Ext} \tag{86}$$

Reactant

Table 77: Properties of each reactant.

Id	Name	SBO
Acetoin	Acetoin	

Modifiers

Table 78: Properties of each modifier.

Id	Name	SBO
Acetoin	Acetoin	
Acetoin_Ext	Acetoin_Ext	

Product

Table 79: Properties of each product.

Id	Name	SBO
Acetoin_Ext	Acetoin_Ext	

Kinetic Law

Derived unit contains undeclared units

$$v_{19} = \text{function\_4\_Acetoin\_transp}([\text{Acetoin}], [\text{Acetoin\_Ext}], \text{Vmax\_Acetoin\_transp}, \text{kmAcetoin\_Acetoin\_transp}, \text{kmAcetoin\_Ext\_Acetoin\_transp}) \quad (87)$$

$$\begin{aligned} &\text{function\_4\_Acetoin\_transp}([\text{Acetoin}], [\text{Acetoin\_Ext}], \text{Vmax\_Acetoin\_transp}, \\ &\quad \text{kmAcetoin\_Acetoin\_transp}, \text{kmAcetoin\_Ext\_Acetoin\_transp}) \\ &= \frac{\text{Vmax\_Acetoin\_transp} \cdot \frac{[\text{Acetoin}]}{\text{kmAcetoin\_Acetoin\_transp}}}{1 + \frac{[\text{Acetoin}]}{\text{kmAcetoin\_Acetoin\_transp}} + \frac{[\text{Acetoin\_Ext}]}{\text{kmAcetoin\_Ext\_Acetoin\_transp}}} \end{aligned} \quad (88)$$

Table 80: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax_Acetoin_transp	Vmax_Acetoin_transp		1.601		☑
kmAcetoin_Acetoin_transp	kmAcetoin_Acetoin_transp		1.893		☑
kmAcetoin_Ext_Acetoin_transp	kmAcetoin_Ext_Acetoin_transp		7.052		☑

6.20 Reaction re32

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

Name Mannitol_transp

Reaction equation

$$\text{Mannitol} \xrightarrow{\text{Mannitol, Mannitol\_Ext}} \text{Mannitol\_Ext} \quad (89)$$

Reactant

Table 81: Properties of each reactant.

Id	Name	SBO
Mannitol	Mannitol	

Modifiers

Table 82: Properties of each modifier.

Id	Name	SBO
Mannitol	Mannitol	
Mannitol_Ext	Mannitol_Ext	

Product

Table 83: Properties of each product.

Id	Name	SBO
Mannitol_Ext	Mannitol_Ext	

Kinetic Law

Derived unit contains undeclared units

$$v_{20} = \text{function\_4\_Mannitol\_transp}([\text{Mannitol}], [\text{Mannitol\_Ext}], \text{Vmax\_Mannitol\_transp}, \text{kmMannitol\_Ext\_Mannitol\_transp}, \text{kmMannitol\_Mannitol\_transp}) \tag{90}$$

$$\begin{aligned} &\text{function\_4\_Mannitol\_transp}([\text{Mannitol}], [\text{Mannitol\_Ext}], \text{Vmax\_Mannitol\_transp}, \\ &\quad \text{kmMannitol\_Ext\_Mannitol\_transp}, \text{kmMannitol\_Mannitol\_transp}) \\ &= \frac{\text{Vmax\_Mannitol\_transp} \cdot \frac{[\text{Mannitol}]}{\text{kmMannitol\_Mannitol\_transp}}}{1 + \frac{[\text{Mannitol}]}{\text{kmMannitol\_Mannitol\_transp}} + \frac{[\text{Mannitol\_Ext}]}{\text{kmMannitol\_Ext\_Mannitol\_transp}}} \end{aligned} \tag{91}$$

Table 84: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax_Mannitol_transp	Vmax_Mannitol_transp		1.625		☑
kmMannitol_Ext_Mannitol_transp	kmMannitol_Ext_Mannitol_transp		0.941		☑
kmMannitol_Mannitol_transp	kmMannitol_Mannitol_transp		0.022		☑

6.21 Reaction re33

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

Name FBPase

Reaction equation

$$\mathrm{FBP} \xrightarrow{\mathrm{F6P,\ FBP,\ Pint}} \mathrm{F6P} + \mathrm{Pint} \tag{92}$$

Reactant

Table 85: Properties of each reactant.

Id	Name	SBO
FBP	FBP	

Modifiers

Table 86: Properties of each modifier.

Id	Name	SBO
F6P	F6P	
FBP	FBP	
Pint	Pint	

Products

Table 87: Properties of each product.

Id	Name	SBO
F6P	F6P	
Pint	Pint	

Kinetic Law

Derived unit contains undeclared units

$$v_{21} = \mathrm{vol}\left(\mathrm{compartment\_1}\right) \cdot \mathrm{function\_4\_FBPase}\left([\mathrm{F6P}], [\mathrm{FBP}], [\mathrm{Pint}], \mathrm{Vmax\_FBPase}, \mathrm{kmF6P\_FBPase}, \mathrm{kmFBP\_FBPase}, \mathrm{kmPint\_FBPase}\right) \tag{93}$$

$$\text{function\_4\_FBPase}([\text{F6P}],[\text{FBP}],[\text{Pint}],\text{Vmax\_FBPase},\text{kmF6P\_FBPase},\text{kmFBP\_FBPase},\text{kmPint\_FBPase}) = \frac{\text{Vmax\_FBPase}\cdot\frac{[\text{FBP}]}{\text{kmFBP\_FBPase}}}{\frac{[\text{FBP}]}{\text{kmFBP\_FBPase}}+\left(1+\frac{[\text{F6P}]}{\text{kmF6P\_FBPase}}\right)\cdot\left(1+\frac{[\text{Pint}]}{\text{kmPint\_FBPase}}\right)} \tag{94}$$

$$\text{function\_4\_FBPase}([\text{F6P}],[\text{FBP}],[\text{Pint}],\text{Vmax\_FBPase},\text{kmF6P\_FBPase},\text{kmFBP\_FBPase},\text{kmPint\_FBPase}) = \frac{\text{Vmax\_FBPase}\cdot\frac{[\text{FBP}]}{\text{kmFBP\_FBPase}}}{\frac{[\text{FBP}]}{\text{kmFBP\_FBPase}}+\left(1+\frac{[\text{F6P}]}{\text{kmF6P\_FBPase}}\right)\cdot\left(1+\frac{[\text{Pint}]}{\text{kmPint\_FBPase}}\right)} \tag{95}$$

Table 88: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmax_FBPase	Vmax_FBPase		0.097		☑
kmF6P_FBPase	kmF6P_FBPase		1.908		☑
kmFBP_FBPase	kmFBP_FBPase		0.412		☑
kmPint-_FBPase	kmPint_FBPase		0.011		☑

7 Derived Rate Equations

When interpreted as an ordinary differential equation framework, this model implies the following set of equations for the rates of change of each species.

Identifiers for kinetic laws highlighted in gray cannot be verified to evaluate to units of SBML `substance` per `time`. As a result, some SBML interpreters may not be able to verify the consistency of the units on quantities in the model. Please check if

- parameters without an unit definition are involved or
- volume correction is necessary because the `hasOnlySubstanceUnits` flag may be set to `false` and `spacialDimensions`> 0 for certain species.

7.1 Species G6P

Name G6P

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

This species takes part in four reactions (as a reactant in re15 and as a product in re12 and as a modifier in re12, re15).

$$\frac{\text{d}}{\text{d}t}\text{G6P} = v_1 - v_4 \tag{96}$$

7.2 Species ATP

Name ATP

Initial concentration $4.88632508879394\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in 14 reactions (as a reactant in re13, re14, re16 and as a product in re20, re21, re25 and as a modifier in re13, re14, re16, re20, re21, re24, re24, re25).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ATP} = v_8 + v_9 + v_{13} - v_2 - v_3 - v_5 \tag{97}$$

7.3 Species ADP

Name ADP

Initial concentration $20.3856905308319\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in eleven reactions (as a reactant in re20, re21, re25 and as a product in re13, re14, re16 and as a modifier in re14, re16, re20, re21, re25).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ADP} = v_2 + v_3 + v_5 - v_8 - v_9 - v_{13} \tag{98}$$

7.4 Species Pint

Name Pint

Initial concentration $38.26\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in 14 reactions (as a reactant in re18 and as a product in re13, re14, re33 and as a modifier in re12, re12, re14, re14, re18, re21, re21, re22, re22, re33).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Pint} = v_2 + 2\,v_3 + v_{21} - v_7 \tag{99}$$

7.5 Species F6P

Name F6P

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

This species takes part in nine reactions (as a reactant in re16, re28 and as a product in re15, re33 and as a modifier in re15, re16, re28, re28, re33).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{F6P} = v_4 + v_{21} - v_5 - v_{16} \tag{100}$$

7.6 Species FBP

Name FBP

Initial concentration $15.3\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in twelve reactions (as a reactant in re17, re33 and as a product in re16 and as a modifier in re12, re12, re16, re17, re21, re21, re22, re22, re33).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{FBP} = v_5 - v_6 - v_{21} \tag{101}$$

7.7 Species G3P

Name G3P

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

This species takes part in six reactions (as a reactant in re18 and as a product in re17 and as a modifier in re17, re18, re23, re23).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{G3P} = 2\,v_6 - v_7 \tag{102}$$

7.8 Species BPG

Name BPG

Initial concentration $1.26348531244692\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in four reactions (as a reactant in re20 and as a product in re18 and as a modifier in re18, re20).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{BPG} = v_7 - v_8 \tag{103}$$

7.9 Species PEP

Name PEP

Initial concentration $2.4790177588998\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in eight reactions (as a reactant in re12, re21, re30 and as a product in re20 and as a modifier in re12, re20, re21, re30).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{PEP} = v_8 - v_1 - v_9 - v_{18} \tag{104}$$

7.10 Species NAD

Name NAD

Initial concentration $4.67\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in ten reactions (as a reactant in re18 and as a product in re22, re24, re27, re28 and as a modifier in re18, re22, re24, re27, re28).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{NAD} = v_{10} + 2\,v_{12} + v_{15} + v_{16} - v_{7} \tag{105}$$

7.11 Species NADH

Name NADH

Initial concentration $2.03337939283534\cdot 10^{-6}\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in ten reactions (as a reactant in re22, re24, re27, re28 and as a product in re18 and as a modifier in re18, re22, re24, re27, re28).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{NADH} = v_{7} - v_{10} - 2\,v_{12} - v_{15} - v_{16} \tag{106}$$

7.12 Species PYR

Name PYR

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

This species takes part in twelve reactions (as a reactant in re22, re23, re26 and as a product in re12, re21, re30 and as a modifier in re12, re21, re22, re23, re26, re30).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{PYR} = v_{1} + v_{9} + v_{18} - v_{10} - v_{11} - 2\,v_{14} \tag{107}$$

7.13 Species AcetCoA

Name AcetCoA

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

This species takes part in six reactions (as a reactant in re24, re25 and as a product in re23 and as a modifier in re23, re24, re25).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{AcetCoA} = v_{11} - v_{12} - v_{13} \tag{108}$$

7.14 Species Acetoin

Name Acetoin

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

This species takes part in six reactions (as a reactant in re27, re31 and as a product in re26 and as a modifier in re26, re27, re31).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Acetoin} = v_{14} - v_{15} - v_{19} \tag{109}$$

7.15 Species Mannitol

Name Mannitol

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

This species takes part in four reactions (as a reactant in re32 and as a product in re29 and as a modifier in re29, re32).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Mannitol} = v_{17} - v_{20} \tag{110}$$

7.16 Species Mannitol1Phosphate

Name Mannitol1Phosphate

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

This species takes part in six reactions (as a reactant in re29 and as a product in re28, re30 and as a modifier in re28, re29, re30).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Mannitol1Phosphate} = v_{16} + v_{18} - v_{17} \tag{111}$$

7.17 Species CoA

Name CoA

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

This species takes part in six reactions (as a reactant in re23 and as a product in re24, re25 and as a modifier in re23, re24, re25).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{CoA} = v_{12} + v_{13} - v_{11} \tag{112}$$

7.18 Species Pext

Name Pext

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

This species takes part in two reactions (as a reactant in re14 and as a modifier in re14).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Pext} = -v_3 \tag{113}$$

7.19 Species Lactate

Name Lactate

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

This species takes part in two reactions (as a product in re22 and as a modifier in re22).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Lactate} = v_{10} \tag{114}$$

7.20 Species Ethanol

Name Ethanol

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

This species takes part in two reactions (as a product in re24 and as a modifier in re24).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Ethanol} = v_{12} \tag{115}$$

7.21 Species Acetate

Name Acetate

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

This species takes part in two reactions (as a product in re25 and as a modifier in re25).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Acetate} = v_{13} \tag{116}$$

7.22 Species Butanediol

Name Butanediol

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

This species takes part in two reactions (as a product in re27 and as a modifier in re27).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Butanediol} = v_{15} \tag{117}$$

7.23 Species Glucose

Name Glucose

Initial concentration $80\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in re12 and as a modifier in re12).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Glucose} = -v_1 \tag{118}$$

7.24 Species Acetoin_Ext

Name Acetoin_Ext

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

This species takes part in two reactions (as a product in re31 and as a modifier in re31).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Acetoin\_Ext} = v_{19} \tag{119}$$

7.25 Species Mannitol_Ext

Name Mannitol_Ext

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

This species takes part in four reactions (as a reactant in re30 and as a product in re32 and as a modifier in re30, re32).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Mannitol\_Ext} = v_{20} - v_{18} \tag{120}$$

7.26 Species Formate

Name Formate

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

This species takes part in two reactions (as a product in re23 and as a modifier in re23).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Formate} = v_{11} \tag{121}$$

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