SBML Model Report

Model name: "Arnold2011_Poolman2000-_CalvinCycle_Starch"

May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by the following three authors: Vijayalakshmi Chelliah[1], Anne Arnold[2] and Zoran Nikoloski[3] at September 16th 2011 at 2:50 p. m. and last time modified at April eighth 2016 at 5:11 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	22
events	0	constraints	0
reactions	21	function definitions	7
global parameters	0	unit definitions	2
rules	2	initial assignments	0

Model Notes

This model is from the article:
A quantitative comparison of CalvinBenson cycle models

[1]EMBL-EBI, viji@ebi.ac.uk
[2]Max-Planck-Institute of Molecular Plant Physiology, arnold@mpimp-golm.mpg.de
[3]Institute of Biochemistry and Biology, University of Potsdam, 14476 Potsdam, Germany, nikoloski@mpimp-golm.mpg.de

Anne Arnold, Zoran Nikoloski Trends in Plant Science2011 Oct 14. 22001849,

Abstract:
The Calvin-Benson cycle (CBC) provides the precursors for biomass synthesis necessary for plant growth. The dynamic behavior and yield of the CBC depend on the environmental conditions and regulation of the cellular state. Accurate quantitative models hold the promise of identifying the key determinants of the tightly regulated CBC function and their effects on the responses in future climates. We provide an integrative analysis of the largest compendium of existing models for photosynthetic processes. Based on the proposed ranking, our framework facilitates the discovery of best-performing models with regard to metabolomics data and of candidates for metabolic engineering.

Note: Model of the Calvin cycle and the related end-product pathway to starch synthesis by Poolman et al. (2000, DOI:10.1093/jexbot/51.suppl_1.319). The parameter values are widely taken from Pettersson and Ryde-Pettersson (1988, DOI:10.1111/j.1432-1033.1988.tb14242.x) and Poolman (1999, [click here for PDF]). The initial metabolite values are chosen from the data set of Zhu et al. (2007, DOI:10.1104/pp.107.103713). A detailed description of all modifications is given in the model described by Arnold and Nikoloski (2011, PMID:22001849.

2 Unit Definitions

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

2.1 Unit `volume`

Definition l

2.2 Unit `substance`

Definition mmol

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
`chloroplast`	chloroplast		3	1	litre	☑	
`cytosol`	cytosol		3	1	litre	☑	

3.1 Compartment `chloroplast`

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

Name chloroplast

3.2 Compartment `cytosol`

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

Name cytosol

4 Species

This model contains 22 species. The boundary condition of six 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
RuBP	RuBP	chloroplast	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☐
PGA	PGA	chloroplast	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☐
DPGA	DPGA	chloroplast	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☐
GAP	GAP	chloroplast	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☐
DHAP	DHAP	chloroplast	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☐
FBP	FBP	chloroplast	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☐
F6P	F6P	chloroplast	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☐
E4P	E4P	chloroplast	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☐
SBP	SBP	chloroplast	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☐
S7P	S7P	chloroplast	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☐
X5P	X5P	chloroplast	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☐
R5P	R5P	chloroplast	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☐
Ru5P	Ru5P	chloroplast	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☐
G6P	G6P	chloroplast	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☐
G1P	G1P	chloroplast	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☐
ATP	ATP	chloroplast	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☐
ADP	ADP	chloroplast	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☑
NADPH	NADPH	chloroplast	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑	☑
NADP	NADP	chloroplast	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑	☑
H	H	chloroplast	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑	☑
Pi	Pi	chloroplast	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☑

Id	Name	Compartment	Derived Unit	Constant	Boundary Condition
Pext	Pext	cytosol	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑	☑

5 Function definitions

This is an overview of seven function definitions.

5.1 Function definition function_2

Name MM s1 + reg 2*c (FBPase)

Arguments Vm, S, K, R1, KR1, R2, KR2

Mathematical Expression

$$\frac{\mathrm{Vm} \cdot \mathrm{S}}{\mathrm{S} + \mathrm{K} \cdot \left(1 + \frac{\mathrm{R1}}{\mathrm{KR1}} + \frac{\mathrm{R2}}{\mathrm{KR2}}\right)} \tag{1}$$

5.2 Function definition function_7

Name MM s1 + reg A,3*c (TPT)

Arguments Vm, S, KA, A, K, R1, KR1, R2, KR2, R3, KR3

Mathematical Expression

$$\frac{\mathrm{Vm} \cdot \mathrm{S}}{\mathrm{S} \cdot \left(1 + \frac{\mathrm{KA}}{\mathrm{A}}\right) + \mathrm{K} \cdot \left(1 + \left(1 + \frac{\mathrm{KA}}{\mathrm{A}}\right) \cdot \left(\frac{\mathrm{R1}}{\mathrm{KR1}} + \frac{\mathrm{R2}}{\mathrm{KR2}} + \frac{\mathrm{R3}}{\mathrm{KR3}}\right)\right)} \tag{2}$$

5.3 Function definition function_4

Name MM s2 + reg 3*c-s1,1*m-s2 (Ru5P kinase)

Arguments Vm, S1, S2, K1, R1, KR1, R2, KR2, R3, KR3, R4, KR41, K2, KR42

Mathematical Expression

$$\frac{\mathrm{Vm} \cdot \mathrm{S1} \cdot \mathrm{S2}}{\left(\mathrm{S1} + \mathrm{K1} \cdot \left(1 + \frac{\mathrm{R1}}{\mathrm{KR1}} + \frac{\mathrm{R2}}{\mathrm{KR2}} + \frac{\mathrm{R3}}{\mathrm{KR3}}\right)\right) \cdot \left(\mathrm{S2} \cdot \left(1 + \frac{\mathrm{R4}}{\mathrm{KR41}}\right) + \mathrm{K2} \cdot \left(1 + \frac{\mathrm{R4}}{\mathrm{KR42}}\right)\right)} \tag{3}$$

5.4 Function definition function_6

Name MM s2 - reg (ATP synth)

Arguments Vm, s1, s2, K1, K2

Mathematical Expression

$$\frac{\mathrm{Vm} \cdot \mathrm{s1} \cdot \mathrm{s2}}{(\mathrm{s1} + \mathrm{K1}) \cdot (\mathrm{s2} + \mathrm{K2})} \tag{4}$$

5.5 Function definition function_1

Name MM s1 + reg 5*c (RuBisCO)

Arguments Vm, S, K, R1, KR1, R2, KR2, R3, KR3, R4, KR4, R5, KR5

Mathematical Expression

$$\frac{\mathrm{Vm}\cdot \mathrm{S}}{\mathrm{S}+\mathrm{K}\cdot\left(1+\frac{\mathrm{R1}}{\mathrm{KR1}}+\frac{\mathrm{R2}}{\mathrm{KR2}}+\frac{\mathrm{R3}}{\mathrm{KR3}}+\frac{\mathrm{R4}}{\mathrm{KR4}}+\frac{\mathrm{R5}}{\mathrm{KR5}}\right)} \tag{5}$$

5.6 Function definition function_3

Name MM s1 + reg 1*c (SBPase, starch phos)

Arguments Vm, S, K, R1, KR1

Mathematical Expression

$$\frac{\mathrm{Vm}\cdot \mathrm{S}}{\mathrm{S}+\mathrm{K}\cdot\left(1+\frac{\mathrm{R1}}{\mathrm{KR1}}\right)} \tag{6}$$

5.7 Function definition function_5

Name starch synthase

Arguments Vm, S1, S2, K1, K2, R1, KR1, R2, KA1, A1, KA2, A2, KA3, A3

Mathematical Expression

$$\frac{\mathrm{Vm}\cdot \mathrm{S1}\cdot \mathrm{S2}}{(\mathrm{S1}+\mathrm{K1})\cdot\left(1+\frac{\mathrm{R1}}{\mathrm{KR1}}\right)\cdot\left(\mathrm{S2}+\mathrm{K2}\cdot\left(1+\frac{\mathrm{K2}\cdot\mathrm{R2}}{\mathrm{KA1}\cdot\mathrm{A1}+\mathrm{KA2}\cdot\mathrm{A2}+\mathrm{KA3}\cdot\mathrm{A3}}\right)\right)} \tag{7}$$

6 Rules

This is an overview of two rules.

6.1 Rule Pi

Rule Pi is an assignment rule for species Pi:

$$\begin{aligned}\mathrm{Pi} = 15 - 2\cdot(&[\mathrm{RuBP}]+[\mathrm{DPGA}]+[\mathrm{FBP}]+[\mathrm{SBP}])-([\mathrm{PGA}]+[\mathrm{GAP}]+[\mathrm{DHAP}]+[\mathrm{F6P}]\\ &+[\mathrm{E4P}]+[\mathrm{S7P}]+[\mathrm{X5P}]+[\mathrm{R5P}]+[\mathrm{Ru5P}]+[\mathrm{G6P}]+[\mathrm{G1P}]+[\mathrm{ATP}])\end{aligned} \tag{8}$$

6.2 Rule ADP

Rule ADP is an assignment rule for species ADP:

$$\mathrm{ADP} = 1.5 - [\mathrm{ATP}] \tag{9}$$

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 4: Overview of all reactions

№	Id	Name	Reaction Equation	SBO
1	RuBisCO	RuBisCo	$\mathrm{RuBP} \xrightarrow{\mathrm{PGA,\ FBP,\ SBP,\ Pi,\ NADPH}} 2\,\mathrm{PGA}$	
2	PGA_K	PGA kinase	$\mathrm{PGA} + \mathrm{ATP} \rightleftharpoons \mathrm{DPGA} + \mathrm{ADP}$	
3	GAP_DH	GAP dehydrogenase	$\mathrm{DPGA} + \mathrm{NADPH} + \mathrm{H} \rightleftharpoons \mathrm{GAP} + \mathrm{NADP} + \mathrm{Pi}$	
4	TP_I	TP isomerase	$\mathrm{GAP} \rightleftharpoons \mathrm{DHAP}$	
5	FBP_A	FBP aldolase	$\mathrm{DHAP} + \mathrm{GAP} \rightleftharpoons \mathrm{FBP}$	
6	FBPase	FBP ase	$\mathrm{FBP} \xrightarrow{\mathrm{F6P,\ Pi}} \mathrm{F6P} + \mathrm{Pi}$	
7	F6P_TK	F6P transketolase	$\mathrm{GAP} + \mathrm{F6P} \rightleftharpoons \mathrm{X5P} + \mathrm{E4P}$	
8	SBP_A	SBP aldolase	$\mathrm{DHAP} + \mathrm{E4P} \rightleftharpoons \mathrm{SBP}$	
9	SBPase	SBP ase	$\mathrm{SBP} \xrightarrow{\mathrm{Pi}} \mathrm{S7P} + \mathrm{Pi}$	
10	S7P_TK	S7P transketolase	$\mathrm{GAP} + \mathrm{S7P} \rightleftharpoons \mathrm{X5P} + \mathrm{R5P}$	
11	R5P_I	R5P isomerase	$\mathrm{R5P} \rightleftharpoons \mathrm{Ru5P}$	
12	Ru5P_E	Ru5P epimerase	$\mathrm{X5P} \rightleftharpoons \mathrm{Ru5P}$	
13	Ru5P_K	Ru5P kinase	$\mathrm{Ru5P} + \mathrm{ATP} \xrightarrow{\mathrm{PGA,\ RuBP,\ Pi,\ ADP}} \mathrm{RuBP} + \mathrm{ADP}$	
14	PG_I	PG isomerase	$\mathrm{F6P} \rightleftharpoons \mathrm{G6P}$	
15	PG_M	PG mutase	$\mathrm{G6P} \rightleftharpoons \mathrm{G1P}$	
16	Starch_S	starch synthase	$\mathrm{G1P} + \mathrm{ATP} \xrightarrow{\mathrm{ADP,\ Pi,\ PGA,\ F6P,\ FBP}} \emptyset$	
17	Starch_P	starch phosphorylase	$\mathrm{Pi} \xrightarrow{\mathrm{G1P}} \mathrm{G1P}$	
18	ATP_S	ATP synthetase	$\mathrm{ADP} + \mathrm{Pi} \longrightarrow \mathrm{ATP}$	
19	TPT_PGA	TPT - PGA	$\mathrm{PGA} \xrightarrow{\mathrm{Pext,\ Pi,\ GAP,\ DHAP}} \emptyset$	

№	Id	Name	Reaction Equation	SBO
20	TPT_GAP	TPT - GAP	$\text{GAP} \xrightarrow{\text{Pext, Pi, PGA, DHAP}} \emptyset$	
21	TPT_DHAP	TPT - DHAP	$\text{DHAP} \xrightarrow{\text{Pext, Pi, PGA, GAP}} \emptyset$	

7.1 Reaction RuBisCO

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

Name RuBisCo

Reaction equation

$$\mathrm{RuBP} \xrightarrow{\mathrm{PGA,\ FBP,\ SBP,\ Pi,\ NADPH}} 2\,\mathrm{PGA} \tag{10}$$

Reactant

Table 5: Properties of each reactant.

Id	Name	SBO
RuBP	RuBP	

Modifiers

Table 6: Properties of each modifier.

Id	Name	SBO
PGA	PGA	
FBP	FBP	
SBP	SBP	
Pi	Pi	
NADPH	NADPH	

Product

Table 7: Properties of each product.

Id	Name	SBO
PGA	PGA	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \mathrm{vol}\,(\mathrm{chloroplast}) \cdot \mathrm{function\_1}\,(\mathrm{Vm}, [\mathrm{RuBP}], \mathrm{K}, [\mathrm{PGA}], \mathrm{KR1}, [\mathrm{FBP}], \mathrm{KR2}, [\mathrm{SBP}], \mathrm{KR3}, [\mathrm{Pi}], \mathrm{KR4}, [\mathrm{NADPH}], \mathrm{KR5}) \tag{11}$$

$$\text{function\_1}\left(\text{Vm},\text{S},\text{K},\text{R1},\text{KR1},\text{R2},\text{KR2},\text{R3},\text{KR3},\text{R4},\text{KR4},\text{R5},\text{KR5}\right) = \frac{\text{Vm}\cdot\text{S}}{\text{S}+\text{K}\cdot\left(1+\frac{\text{R1}}{\text{KR1}}+\frac{\text{R2}}{\text{KR2}}+\frac{\text{R3}}{\text{KR3}}+\frac{\text{R4}}{\text{KR4}}+\frac{\text{R5}}{\text{KR5}}\right)} \tag{12}$$

$$\text{function\_1}\left(\text{Vm},\text{S},\text{K},\text{R1},\text{KR1},\text{R2},\text{KR2},\text{R3},\text{KR3},\text{R4},\text{KR4},\text{R5},\text{KR5}\right) = \frac{\text{Vm}\cdot\text{S}}{\text{S}+\text{K}\cdot\left(1+\frac{\text{R1}}{\text{KR1}}+\frac{\text{R2}}{\text{KR2}}+\frac{\text{R3}}{\text{KR3}}+\frac{\text{R4}}{\text{KR4}}+\frac{\text{R5}}{\text{KR5}}\right)} \tag{13}$$

Table 8: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vm	Vm	0000009	340.000		☑
K	K	0000009	0.020		☑
KR1	KR1	0000009	0.840		☑
KR2	KR2	0000009	0.040		☑
KR3	KR3	0000009	0.008		☑
KR4	KR4	0000009	0.900		☑
KR5	KR5	0000009	0.070		☑

7.2 Reaction PGA_K

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

Name PGA kinase

Reaction equation

$$\text{PGA} + \text{ATP} \rightleftharpoons \text{DPGA} + \text{ADP} \tag{14}$$

Reactants

Table 9: Properties of each reactant.

Id	Name	SBO
PGA	PGA	
ATP	ATP	

Products

Table 10: Properties of each product.

Id	Name	SBO
DPGA	DPGA	
ADP	ADP	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \mathrm{vol}\,(\mathrm{chloroplast}) \cdot (\mathrm{k1} \cdot [\mathrm{PGA}] \cdot [\mathrm{ATP}] - \mathrm{k2} \cdot [\mathrm{DPGA}] \cdot [\mathrm{ADP}]) \tag{15}$$

Table 11: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1	0000009	$5 \cdot 10^{8}$		☑
k2	k2	0000009	$1.6129 \cdot 10^{12}$		☑

7.3 Reaction GAP_DH

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

Name GAP dehydrogenase

Reaction equation

$$\mathrm{DPGA} + \mathrm{NADPH} + \mathrm{H} \rightleftharpoons \mathrm{GAP} + \mathrm{NADP} + \mathrm{Pi} \tag{16}$$

Reactants

Table 12: Properties of each reactant.

Id	Name	SBO
DPGA	DPGA	
NADPH	NADPH	
H	H	

Products

Table 13: Properties of each product.

Id	Name	SBO
GAP	GAP	
NADP	NADP	
Pi	Pi	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \text{vol}\,(\text{chloroplast}) \cdot (\text{k1} \cdot [\text{DPGA}] \cdot [\text{NADPH}] \cdot [\text{H}] - \text{k2} \cdot [\text{GAP}] \cdot [\text{NADP}] \cdot [\text{Pi}]) \quad (17)$$

Table 14: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1	0000009	$5 \cdot 10^8$		☑
k2	k2	0000009	31.250		☑

7.4 Reaction TP_I

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

Name TP isomerase

Reaction equation

$$\text{GAP} \rightleftharpoons \text{DHAP} \quad (18)$$

Reactant

Table 15: Properties of each reactant.

Id	Name	SBO
GAP	GAP	

Product

Table 16: Properties of each product.

Id	Name	SBO
DHAP	DHAP	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \mathrm{vol}\,(\mathrm{chloroplast}) \cdot (\mathrm{k1} \cdot [\mathrm{GAP}] - \mathrm{k2} \cdot [\mathrm{DHAP}]) \tag{19}$$

Table 17: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1	0000009	$5 \cdot 10^8$		☑
k2	k2	0000009	$2.2727 \cdot 10^7$		☑

7.5 Reaction FBP_A

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

Name FBP aldolase

Reaction equation

$$\mathrm{DHAP} + \mathrm{GAP} \rightleftharpoons \mathrm{FBP} \tag{20}$$

Reactants

Table 18: Properties of each reactant.

Id	Name	SBO
DHAP	DHAP	
GAP	GAP	

Product

Table 19: Properties of each product.

Id	Name	SBO
FBP	FBP	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \mathrm{vol}\,(\mathrm{chloroplast}) \cdot (\mathrm{k1} \cdot [\mathrm{DHAP}] \cdot [\mathrm{GAP}] - \mathrm{k2} \cdot [\mathrm{FBP}]) \tag{21}$$

Table 20: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1	0000009	$5 \cdot 10^8$		☑
k2	k2	0000009	$7.0423 \cdot 10^7$		☑

7.6 Reaction FBPase

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

Name FBP ase

Reaction equation

$$\mathrm{FBP} \xrightarrow{\mathrm{F6P,\ Pi}} \mathrm{F6P} + \mathrm{Pi} \tag{22}$$

Reactant

Table 21: Properties of each reactant.

Id	Name	SBO
FBP	FBP	

Modifiers

Table 22: Properties of each modifier.

Id	Name	SBO
F6P	F6P	
Pi	Pi	

Products

Table 23: Properties of each product.

Id	Name	SBO
F6P	F6P	
Pi	Pi	

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \mathrm{vol}\,(\mathrm{chloroplast}) \cdot \mathrm{function\_2}\,(\mathrm{Vm}, [\mathrm{FBP}], \mathrm{K}, [\mathrm{F6P}], \mathrm{KR1}, [\mathrm{Pi}], \mathrm{KR2}) \tag{23}$$

$$\mathrm{function\_2}\,(\mathrm{Vm}, \mathrm{S}, \mathrm{K}, \mathrm{R1}, \mathrm{KR1}, \mathrm{R2}, \mathrm{KR2}) = \frac{\mathrm{Vm} \cdot \mathrm{S}}{\mathrm{S} + \mathrm{K} \cdot \left(1 + \frac{\mathrm{R1}}{\mathrm{KR1}} + \frac{\mathrm{R2}}{\mathrm{KR2}}\right)} \tag{24}$$

$$\mathrm{function\_2}\,(\mathrm{Vm}, \mathrm{S}, \mathrm{K}, \mathrm{R1}, \mathrm{KR1}, \mathrm{R2}, \mathrm{KR2}) = \frac{\mathrm{Vm} \cdot \mathrm{S}}{\mathrm{S} + \mathrm{K} \cdot \left(1 + \frac{\mathrm{R1}}{\mathrm{KR1}} + \frac{\mathrm{R2}}{\mathrm{KR2}}\right)} \tag{25}$$

Table 24: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vm	Vm	0000009	200.00		☑
K	K	0000009	0.03		☑
KR1	KR1	0000009	0.70		☑
KR2	KR2	0000009	12.00		☑

7.7 Reaction F6P_TK

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

Name F6P transketolase

Reaction equation

$$\mathrm{GAP} + \mathrm{F6P} \rightleftharpoons \mathrm{X5P} + \mathrm{E4P} \tag{26}$$

Reactants

Table 25: Properties of each reactant.

Id	Name	SBO
GAP	GAP	
F6P	F6P	

Products

Table 26: Properties of each product.

Id	Name	SBO
X5P	X5P	
E4P	E4P	

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \mathrm{vol}\,(\mathrm{chloroplast}) \cdot (\mathrm{k1} \cdot [\mathrm{GAP}] \cdot [\mathrm{F6P}] - \mathrm{k2} \cdot [\mathrm{X5P}] \cdot [\mathrm{E4P}]) \tag{27}$$

Table 27: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1	0000009	$5 \cdot 10^8$		☑
k2	k2	0000009	$5.9524 \cdot 10^9$		☑

7.8 Reaction SBP_A

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

Name SBP aldolase

Reaction equation

$$\mathrm{DHAP} + \mathrm{E4P} \rightleftharpoons \mathrm{SBP} \tag{28}$$

Reactants

Table 28: Properties of each reactant.

Id	Name	SBO
DHAP	DHAP	
E4P	E4P	

Product

Table 29: Properties of each product.

Id	Name	SBO
SBP	SBP	

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \text{vol}\,(\text{chloroplast}) \cdot (\text{k1} \cdot [\text{DHAP}] \cdot [\text{E4P}] - \text{k2} \cdot [\text{SBP}]) \tag{29}$$

Table 30: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1	0000009	$5 \cdot 10^8$		☑
k2	k2	0000009	$3.84615 \cdot 10^7$		☑

7.9 Reaction SBPase

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

Name SBP ase

Reaction equation

$$\text{SBP} \xrightarrow{\text{Pi}} \text{S7P} + \text{Pi} \tag{30}$$

Reactant

Table 31: Properties of each reactant.

Id	Name	SBO
SBP	SBP	

Modifier

Table 32: Properties of each modifier.

Id	Name	SBO
Pi	Pi	

Products

Table 33: Properties of each product.

Id	Name	SBO
S7P	S7P	
Pi	Pi	

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \text{vol}\left(\text{chloroplast}\right) \cdot \text{function\_3}\left(\text{Vm}, [\text{SBP}], \text{K}, [\text{Pi}], \text{KR1}\right) \tag{31}$$

$$\text{function\_3}\left(\text{Vm}, \text{S}, \text{K}, \text{R1}, \text{KR1}\right) = \frac{\text{Vm} \cdot \text{S}}{\text{S} + \text{K} \cdot \left(1 + \frac{\text{R1}}{\text{KR1}}\right)} \tag{32}$$

$$\text{function\_3}\left(\text{Vm}, \text{S}, \text{K}, \text{R1}, \text{KR1}\right) = \frac{\text{Vm} \cdot \text{S}}{\text{S} + \text{K} \cdot \left(1 + \frac{\text{R1}}{\text{KR1}}\right)} \tag{33}$$

Table 34: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vm	Vm	0000009	40.00		☑
K	K	0000009	0.02		☑
KR1	KR1	0000009	12.00		☑

7.10 Reaction S7P_TK

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

Name S7P transketolase

Reaction equation

$$\mathrm{GAP} + \mathrm{S7P} \rightleftharpoons \mathrm{X5P} + \mathrm{R5P} \tag{34}$$

Reactants

Table 35: Properties of each reactant.

Id	Name	SBO
GAP	GAP	
S7P	S7P	

Products

Table 36: Properties of each product.

Id	Name	SBO
X5P	X5P	
R5P	R5P	

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = \mathrm{vol}\,(\mathrm{chloroplast}) \cdot (\mathrm{k1} \cdot [\mathrm{GAP}] \cdot [\mathrm{S7P}] - \mathrm{k2} \cdot [\mathrm{X5P}] \cdot [\mathrm{R5P}]) \tag{35}$$

Table 37: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1	0000009	$5 \cdot 10^8$		☑
k2	k2	0000009	$5.8824 \cdot 10^8$		☑

7.11 Reaction R5P_I

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

Name R5P isomerase

Reaction equation

$$\mathrm{R5P} \rightleftharpoons \mathrm{Ru5P} \tag{36}$$

Reactant

Table 38: Properties of each reactant.

Id	Name	SBO
R5P	R5P	

Product

Table 39: Properties of each product.

Id	Name	SBO
Ru5P	Ru5P	

Kinetic Law

Derived unit contains undeclared units

$$v_{11} = \mathrm{vol}\,(\mathrm{chloroplast}) \cdot (\mathrm{k1} \cdot [\mathrm{R5P}] - \mathrm{k2} \cdot [\mathrm{Ru5P}]) \tag{37}$$

Table 40: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1	0000009	$5 \cdot 10^{8}$		☑
k2	k2	0000009	$1.25 \cdot 10^{9}$		☑

7.12 Reaction Ru5P_E

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

Name Ru5P epimerase

Reaction equation

$$\mathrm{X5P} \rightleftharpoons \mathrm{Ru5P} \tag{38}$$

Reactant

Table 41: Properties of each reactant.

Id	Name	SBO
X5P	X5P	

Product

Table 42: Properties of each product.

Id	Name	SBO
Ru5P	Ru5P	

Kinetic Law

Derived unit contains undeclared units

$$v_{12} = \mathrm{vol}\,(\mathrm{chloroplast}) \cdot (\mathrm{k1} \cdot [\mathrm{X5P}] - \mathrm{k2} \cdot [\mathrm{Ru5P}]) \tag{39}$$

Table 43: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1	0000009	$5 \cdot 10^8$		☑
k2	k2	0000009	$7.46269 \cdot 10^8$		☑

7.13 Reaction Ru5P_K

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

Name Ru5P kinase

Reaction equation

$$\mathrm{Ru5P} + \mathrm{ATP} \xrightarrow{\mathrm{PGA,\ RuBP,\ Pi,\ ADP}} \mathrm{RuBP} + \mathrm{ADP} \tag{40}$$

Reactants

Table 44: Properties of each reactant.

Id	Name	SBO
Ru5P	Ru5P	

Id	Name	SBO
ATP	ATP	

Modifiers

Table 45: Properties of each modifier.

Id	Name	SBO
PGA	PGA	
RuBP	RuBP	
Pi	Pi	
ADP	ADP	

Products

Table 46: Properties of each product.

Id	Name	SBO
RuBP	RuBP	
ADP	ADP	

Kinetic Law

Derived unit contains undeclared units

$$v_{13} = \mathrm{vol}\left(\mathrm{chloroplast}\right) \cdot \mathrm{function\_4}\left(\mathrm{Vm}, [\mathrm{Ru5P}], [\mathrm{ATP}], \mathrm{K1}, [\mathrm{PGA}], \mathrm{KR1}, [\mathrm{RuBP}], \mathrm{KR2}, [\mathrm{Pi}], \mathrm{KR3}, [\mathrm{ADP}], \mathrm{KR41}, \mathrm{K2}, \mathrm{KR42}\right) \tag{41}$$

$$\mathrm{function\_4}\left(\mathrm{Vm}, \mathrm{S1}, \mathrm{S2}, \mathrm{K1}, \mathrm{R1}, \mathrm{KR1}, \mathrm{R2}, \mathrm{KR2}, \mathrm{R3}, \mathrm{KR3}, \mathrm{R4}, \mathrm{KR41}, \mathrm{K2}, \mathrm{KR42}\right) = \frac{\mathrm{Vm} \cdot \mathrm{S1} \cdot \mathrm{S2}}{\left(\mathrm{S1} + \mathrm{K1} \cdot \left(1 + \frac{\mathrm{R1}}{\mathrm{KR1}} + \frac{\mathrm{R2}}{\mathrm{KR2}} + \frac{\mathrm{R3}}{\mathrm{KR3}}\right)\right) \cdot \left(\mathrm{S2} \cdot \left(1 + \frac{\mathrm{R4}}{\mathrm{KR41}}\right) + \mathrm{K2} \cdot \left(1 + \frac{\mathrm{R4}}{\mathrm{KR42}}\right)\right)} \tag{42}$$

$$\mathrm{function\_4}\left(\mathrm{Vm}, \mathrm{S1}, \mathrm{S2}, \mathrm{K1}, \mathrm{R1}, \mathrm{KR1}, \mathrm{R2}, \mathrm{KR2}, \mathrm{R3}, \mathrm{KR3}, \mathrm{R4}, \mathrm{KR41}, \mathrm{K2}, \mathrm{KR42}\right) = \frac{\mathrm{Vm} \cdot \mathrm{S1} \cdot \mathrm{S2}}{\left(\mathrm{S1} + \mathrm{K1} \cdot \left(1 + \frac{\mathrm{R1}}{\mathrm{KR1}} + \frac{\mathrm{R2}}{\mathrm{KR2}} + \frac{\mathrm{R3}}{\mathrm{KR3}}\right)\right) \cdot \left(\mathrm{S2} \cdot \left(1 + \frac{\mathrm{R4}}{\mathrm{KR41}}\right) + \mathrm{K2} \cdot \left(1 + \frac{\mathrm{R4}}{\mathrm{KR42}}\right)\right)} \tag{43}$$

Table 47: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vm	Vm	0000009	1000.00		☑
K1	K1	0000009	0.05		☑
KR1	KR1	0000009	2.00		☑
KR2	KR2	0000009	0.70		☑
KR3	KR3	0000009	4.00		☑
KR41	KR41	0000009	2.50		☑
K2	K2	0000009	0.05		☑
KR42	KR42	0000009	0.40		☑

7.14 Reaction PG_I

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

Name PG isomerase

Reaction equation

$$\mathrm{F6P} \rightleftharpoons \mathrm{G6P} \tag{44}$$

Reactant

Table 48: Properties of each reactant.

Id	Name	SBO
F6P	F6P	

Product

Table 49: Properties of each product.

Id	Name	SBO
G6P	G6P	

Kinetic Law

Derived unit contains undeclared units

$$v_{14} = \mathrm{vol}\,(\mathrm{chloroplast}) \cdot (\mathrm{k1} \cdot [\mathrm{F6P}] - \mathrm{k2} \cdot [\mathrm{G6P}]) \tag{45}$$

Table 50: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1	0000009	$5 \cdot 10^{8}$		☑
k2	k2	0000009	$2.174 \cdot 10^{8}$		☑

7.15 Reaction PG_M

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

Name PG mutase

Reaction equation

$$\mathrm{G6P} \rightleftharpoons \mathrm{G1P} \tag{46}$$

Reactant

Table 51: Properties of each reactant.

Id	Name	SBO
G6P	G6P	

Product

Table 52: Properties of each product.

Id	Name	SBO
G1P	G1P	

Kinetic Law

Derived unit contains undeclared units

$$v_{15} = \mathrm{vol}\,(\mathrm{chloroplast}) \cdot (\mathrm{k1} \cdot [\mathrm{G6P}] - \mathrm{k2} \cdot [\mathrm{G1P}]) \tag{47}$$

Table 53: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1	0000009	$5 \cdot 10^{8}$		☑
k2	k2	0000009	$8.621 \cdot 10^{9}$		☑

7.16 Reaction Starch_S

This is an irreversible reaction of two reactants forming no product influenced by five modifiers.

Name starch synthase

Notes changed velocity in accordance with the authors: (...)/(G1P+Km1)((1+[ADP]/Ki)([ATP]+Km2*(...)))

Reaction equation

$$\mathrm{G1P} + \mathrm{ATP} \xrightarrow{\mathrm{ADP,\ Pi,\ PGA,\ F6P,\ FBP}} \emptyset \tag{48}$$

Reactants

Table 54: Properties of each reactant.

Id	Name	SBO
G1P	G1P	
ATP	ATP	

Modifiers

Table 55: Properties of each modifier.

Id	Name	SBO
ADP	ADP	
Pi	Pi	
PGA	PGA	
F6P	F6P	
FBP	FBP	

Kinetic Law

Derived unit contains undeclared units

$$v_{16} = \mathrm{vol}\left(\mathrm{chloroplast}\right) \cdot \mathrm{function\_5}\left(\mathrm{Vm}, [\mathrm{G1P}], [\mathrm{ATP}], \mathrm{K1}, \mathrm{K2}, [\mathrm{ADP}], \mathrm{KR1}, [\mathrm{Pi}], \mathrm{KA1}, [\mathrm{PGA}], \mathrm{KA2}, [\mathrm{F6P}], \mathrm{KA3}, [\mathrm{FBP}]\right) \tag{49}$$

$$\begin{aligned} &\mathrm{function\_5}\left(\mathrm{Vm}, \mathrm{S1}, \mathrm{S2}, \mathrm{K1}, \mathrm{K2}, \mathrm{R1}, \mathrm{KR1}, \mathrm{R2}, \mathrm{KA1}, \mathrm{A1}, \mathrm{KA2}, \mathrm{A2}, \mathrm{KA3}, \mathrm{A3}\right) \\ &= \frac{\mathrm{Vm} \cdot \mathrm{S1} \cdot \mathrm{S2}}{(\mathrm{S1} + \mathrm{K1}) \cdot \left(1 + \frac{\mathrm{R1}}{\mathrm{KR1}}\right) \cdot \left(\mathrm{S2} + \mathrm{K2} \cdot \left(1 + \frac{\mathrm{K2 \cdot R2}}{\mathrm{KA1 \cdot A1 + KA2 \cdot A2 + KA3 \cdot A3}}\right)\right)} \end{aligned} \tag{50}$$

$$\begin{aligned}&\text{function\_5}\left(\mathrm{Vm},\mathrm{S1},\mathrm{S2},\mathrm{K1},\mathrm{K2},\mathrm{R1},\mathrm{KR1},\mathrm{R2},\mathrm{KA1},\mathrm{A1},\mathrm{KA2},\mathrm{A2},\mathrm{KA3},\mathrm{A3}\right)\\&=\frac{\mathrm{Vm}\cdot\mathrm{S1}\cdot\mathrm{S2}}{(\mathrm{S1}+\mathrm{K1})\cdot\left(1+\frac{\mathrm{R1}}{\mathrm{KR1}}\right)\cdot\left(\mathrm{S2}+\mathrm{K2}\cdot\left(1+\frac{\mathrm{K2}\cdot\mathrm{R2}}{\mathrm{KA1}\cdot\mathrm{A1}+\mathrm{KA2}\cdot\mathrm{A2}+\mathrm{KA3}\cdot\mathrm{A3}}\right)\right)}\end{aligned}\tag{51}$$

Table 56: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vm	Vm	0000009	40.00		☑
K1	K1	0000009	0.08		☑
K2	K2	0000009	0.08		☑
KR1	KR1	0000009	10.00		☑
KA1	KA1	0000009	0.10		☑
KA2	KA2	0000009	0.02		☑
KA3	KA3	0000009	0.02		☑

7.17 Reaction Starch_P

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

Name starch phosphorylase

Notes Poolman (1999)

Reaction equation

$$\mathrm{Pi}\xrightarrow{\mathrm{G1P}}\mathrm{G1P}\tag{52}$$

Reactant

Table 57: Properties of each reactant.

Id	Name	SBO
Pi	Pi	

Modifier

Table 58: Properties of each modifier.

Id	Name	SBO
G1P	G1P	

Product

Table 59: Properties of each product.

Id	Name	SBO
G1P	G1P	

Kinetic Law

Derived unit contains undeclared units

$$v_{17} = \mathrm{vol}\,(\mathrm{chloroplast}) \cdot \mathrm{function\_3}\,(\mathrm{Vm}, [\mathrm{Pi}], \mathrm{K}, [\mathrm{G1P}], \mathrm{KR1}) \tag{53}$$

$$\mathrm{function\_3}\,(\mathrm{Vm}, \mathrm{S}, \mathrm{K}, \mathrm{R1}, \mathrm{KR1}) = \frac{\mathrm{Vm} \cdot \mathrm{S}}{\mathrm{S} + \mathrm{K} \cdot \left(1 + \frac{\mathrm{R1}}{\mathrm{KR1}}\right)} \tag{54}$$

$$\mathrm{function\_3}\,(\mathrm{Vm}, \mathrm{S}, \mathrm{K}, \mathrm{R1}, \mathrm{KR1}) = \frac{\mathrm{Vm} \cdot \mathrm{S}}{\mathrm{S} + \mathrm{K} \cdot \left(1 + \frac{\mathrm{R1}}{\mathrm{KR1}}\right)} \tag{55}$$

Table 60: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vm	Vm	0000009	40.00		☑
K	K	0000009	0.10		☑
KR1	KR1	0000009	0.05		☑

7.18 Reaction ATP_S

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

Name ATP synthetase

Reaction equation

$$\mathrm{ADP} + \mathrm{Pi} \longrightarrow \mathrm{ATP} \tag{56}$$

Reactants

Table 61: Properties of each reactant.

Id	Name	SBO
ADP	ADP	
Pi	Pi	

Product

Table 62: Properties of each product.

Id	Name	SBO
ATP	ATP	

Kinetic Law

Derived unit contains undeclared units

$$v_{18} = \text{vol}\,(\text{chloroplast}) \cdot \text{function\_6}\,(\text{Vm}, [\text{ADP}], [\text{Pi}], \text{K1}, \text{K2}) \tag{57}$$

$$\text{function\_6}\,(\text{Vm}, \text{s1}, \text{s2}, \text{K1}, \text{K2}) = \frac{\text{Vm} \cdot \text{s1} \cdot \text{s2}}{(\text{s1} + \text{K1}) \cdot (\text{s2} + \text{K2})} \tag{58}$$

$$\text{function\_6}\,(\text{Vm}, \text{s1}, \text{s2}, \text{K1}, \text{K2}) = \frac{\text{Vm} \cdot \text{s1} \cdot \text{s2}}{(\text{s1} + \text{K1}) \cdot (\text{s2} + \text{K2})} \tag{59}$$

Table 63: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vm	Vm	0000009	350.000		☑
K1	K1	0000009	0.014		☑
K2	K2		0.300		☑

7.19 Reaction TPT_PGA

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

Name TPT - PGA

Reaction equation

$$\text{PGA} \xrightarrow{\text{Pext, Pi, GAP, DHAP}} \emptyset \tag{60}$$

Reactant

Table 64: Properties of each reactant.

Id	Name	SBO
PGA	PGA	

Modifiers

Table 65: Properties of each modifier.

Id	Name	SBO
Pext	Pext	
Pi	Pi	
GAP	GAP	
DHAP	DHAP	

Kinetic Law

Derived unit contains undeclared units

$$v_{19} = \mathrm{vol}\,(\mathrm{chloroplast}) \cdot \mathrm{function\_7}\,(\mathrm{Vm}, [\mathrm{PGA}], \mathrm{KA}, [\mathrm{Pext}], \mathrm{K}, [\mathrm{Pi}], \mathrm{KR1}, [\mathrm{GAP}], \mathrm{KR2}, [\mathrm{DHAP}], \mathrm{KR3}) \tag{61}$$

$$\mathrm{function\_7}\,(\mathrm{Vm}, \mathrm{S}, \mathrm{KA}, \mathrm{A}, \mathrm{K}, \mathrm{R1}, \mathrm{KR1}, \mathrm{R2}, \mathrm{KR2}, \mathrm{R3}, \mathrm{KR3}) = \frac{\mathrm{Vm} \cdot \mathrm{S}}{\mathrm{S} \cdot \left(1 + \frac{\mathrm{KA}}{\mathrm{A}}\right) + \mathrm{K} \cdot \left(1 + \left(1 + \frac{\mathrm{KA}}{\mathrm{A}}\right) \cdot \left(\frac{\mathrm{R1}}{\mathrm{KR1}} + \frac{\mathrm{R2}}{\mathrm{KR2}} + \frac{\mathrm{R3}}{\mathrm{KR3}}\right)\right)} \tag{62}$$

$$\mathrm{function\_7}\,(\mathrm{Vm}, \mathrm{S}, \mathrm{KA}, \mathrm{A}, \mathrm{K}, \mathrm{R1}, \mathrm{KR1}, \mathrm{R2}, \mathrm{KR2}, \mathrm{R3}, \mathrm{KR3}) = \frac{\mathrm{Vm} \cdot \mathrm{S}}{\mathrm{S} \cdot \left(1 + \frac{\mathrm{KA}}{\mathrm{A}}\right) + \mathrm{K} \cdot \left(1 + \left(1 + \frac{\mathrm{KA}}{\mathrm{A}}\right) \cdot \left(\frac{\mathrm{R1}}{\mathrm{KR1}} + \frac{\mathrm{R2}}{\mathrm{KR2}} + \frac{\mathrm{R3}}{\mathrm{KR3}}\right)\right)} \tag{63}$$

Table 66: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vm	Vm		250.000		☑
KA	KA		0.740		☑
K	K		0.250		☑
KR1	KR1		0.630		☑
KR2	KR2		0.075		☑
KR3	KR3		0.077		☑

7.20 Reaction TPT_GAP

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

Name TPT - GAP

Reaction equation

$$\mathrm{GAP} \xrightarrow{\mathrm{Pext,\ Pi,\ PGA,\ DHAP}} \emptyset \tag{64}$$

Reactant

Table 67: Properties of each reactant.

Id	Name	SBO
GAP	GAP	

Modifiers

Table 68: Properties of each modifier.

Id	Name	SBO
Pext	Pext	
Pi	Pi	
PGA	PGA	
DHAP	DHAP	

Kinetic Law

Derived unit contains undeclared units

$$\begin{aligned} v_{20} = {} & \mathrm{vol}\left(\mathrm{chloroplast}\right) \\ & \cdot \mathrm{function\_7}\left(\mathrm{Vm}, [\mathrm{GAP}], \mathrm{KA}, [\mathrm{Pext}], \mathrm{K}, [\mathrm{Pi}], \mathrm{KR1}, [\mathrm{PGA}], \mathrm{KR2}, [\mathrm{DHAP}], \mathrm{KR3}\right) \end{aligned} \tag{65}$$

$$\begin{aligned} & \mathrm{function\_7}\left(\mathrm{Vm}, \mathrm{S}, \mathrm{KA}, \mathrm{A}, \mathrm{K}, \mathrm{R1}, \mathrm{KR1}, \mathrm{R2}, \mathrm{KR2}, \mathrm{R3}, \mathrm{KR3}\right) \\ & = \frac{\mathrm{Vm} \cdot \mathrm{S}}{\mathrm{S} \cdot \left(1 + \frac{\mathrm{KA}}{\mathrm{A}}\right) + \mathrm{K} \cdot \left(1 + \left(1 + \frac{\mathrm{KA}}{\mathrm{A}}\right) \cdot \left(\frac{\mathrm{R1}}{\mathrm{KR1}} + \frac{\mathrm{R2}}{\mathrm{KR2}} + \frac{\mathrm{R3}}{\mathrm{KR3}}\right)\right)} \end{aligned} \tag{66}$$

$$\begin{aligned} & \mathrm{function\_7}\left(\mathrm{Vm}, \mathrm{S}, \mathrm{KA}, \mathrm{A}, \mathrm{K}, \mathrm{R1}, \mathrm{KR1}, \mathrm{R2}, \mathrm{KR2}, \mathrm{R3}, \mathrm{KR3}\right) \\ & = \frac{\mathrm{Vm} \cdot \mathrm{S}}{\mathrm{S} \cdot \left(1 + \frac{\mathrm{KA}}{\mathrm{A}}\right) + \mathrm{K} \cdot \left(1 + \left(1 + \frac{\mathrm{KA}}{\mathrm{A}}\right) \cdot \left(\frac{\mathrm{R1}}{\mathrm{KR1}} + \frac{\mathrm{R2}}{\mathrm{KR2}} + \frac{\mathrm{R3}}{\mathrm{KR3}}\right)\right)} \end{aligned} \tag{67}$$

Table 69: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vm	Vm		250.000		☑
KA	KA		0.740		☑
K	K		0.075		☑
KR1	KR1	0000009	0.630		☑
KR2	KR2		0.250		☑
KR3	KR3	0000009	0.077		☑

7.21 Reaction TPT_DHAP

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

Name TPT - DHAP

Reaction equation

$$\mathrm{DHAP} \xrightarrow{\text{Pext, Pi, PGA, GAP}} \emptyset \tag{68}$$

Reactant

Table 70: Properties of each reactant.

Id	Name	SBO
DHAP	DHAP	

Modifiers

Table 71: Properties of each modifier.

Id	Name	SBO
Pext	Pext	
Pi	Pi	
PGA	PGA	
GAP	GAP	

Kinetic Law

Derived unit contains undeclared units

$$v_{21} = \mathrm{vol}\,(\mathrm{chloroplast}) \cdot \mathrm{function\_7}\,(\mathrm{Vm}, [\mathrm{DHAP}], \mathrm{KA}, [\mathrm{Pext}], \mathrm{K}, [\mathrm{Pi}], \mathrm{KR1}, [\mathrm{PGA}], \mathrm{KR2}, [\mathrm{GAP}], \mathrm{KR3}) \tag{69}$$

$$\mathrm{function\_7}\,(\mathrm{Vm}, \mathrm{S}, \mathrm{KA}, \mathrm{A}, \mathrm{K}, \mathrm{R1}, \mathrm{KR1}, \mathrm{R2}, \mathrm{KR2}, \mathrm{R3}, \mathrm{KR3}) = \frac{\mathrm{Vm} \cdot \mathrm{S}}{\mathrm{S} \cdot \left(1 + \frac{\mathrm{KA}}{\mathrm{A}}\right) + \mathrm{K} \cdot \left(1 + \left(1 + \frac{\mathrm{KA}}{\mathrm{A}}\right) \cdot \left(\frac{\mathrm{R1}}{\mathrm{KR1}} + \frac{\mathrm{R2}}{\mathrm{KR2}} + \frac{\mathrm{R3}}{\mathrm{KR3}}\right)\right)} \tag{70}$$

$$\mathrm{function\_7}\,(\mathrm{Vm}, \mathrm{S}, \mathrm{KA}, \mathrm{A}, \mathrm{K}, \mathrm{R1}, \mathrm{KR1}, \mathrm{R2}, \mathrm{KR2}, \mathrm{R3}, \mathrm{KR3}) = \frac{\mathrm{Vm} \cdot \mathrm{S}}{\mathrm{S} \cdot \left(1 + \frac{\mathrm{KA}}{\mathrm{A}}\right) + \mathrm{K} \cdot \left(1 + \left(1 + \frac{\mathrm{KA}}{\mathrm{A}}\right) \cdot \left(\frac{\mathrm{R1}}{\mathrm{KR1}} + \frac{\mathrm{R2}}{\mathrm{KR2}} + \frac{\mathrm{R3}}{\mathrm{KR3}}\right)\right)} \tag{71}$$

Table 72: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vm	Vm		250.000		☑
KA	KA		0.740		☑
K	K		0.077		☑
KR1	KR1		0.630		☑
KR2	KR2		0.250		☑
KR3	KR3		0.075		☑

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 RuBP

Name RuBP

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

This species takes part in three reactions (as a reactant in RuBisCO and as a product in Ru5P_K and as a modifier in Ru5P_K).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{RuBP} = v_{13} - v_1 \tag{72}$$

8.2 Species PGA

Name PGA

Initial concentration $2.4\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in eight reactions (as a reactant in PGA_K, TPT_PGA and as a product in RuBisCO and as a modifier in RuBisCO, Ru5P_K, Starch_S, TPT_GAP, TPT_DHAP).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{PGA} = 2\,v_1 - v_2 - v_{19} \tag{73}$$

8.3 Species DPGA

Name DPGA

Initial concentration $0.0011\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in GAP_DH and as a product in PGA_K).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{DPGA} = v_2 - v_3 \tag{74}$$

8.4 Species GAP

Name GAP

Initial concentration $0.02\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in eight reactions (as a reactant in TP_I, FBP_A, F6P_TK, S7P_TK, TPT_GAP and as a product in GAP_DH and as a modifier in TPT_PGA, TPT_DHAP).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{GAP} = v_3 - v_4 - v_5 - v_7 - v_{10} - v_{20} \tag{75}$$

8.5 Species DHAP

Name DHAP

Initial concentration $0.48\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in six reactions (as a reactant in FBP_A, SBP_A, TPT_DHAP and as a product in TP_I and as a modifier in TPT_PGA, TPT_GAP).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{DHAP} = v_4 - v_5 - v_8 - v_{21} \tag{76}$$

8.6 Species FBP

Name FBP

Initial concentration $0.669999999999999\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in four reactions (as a reactant in FBPase and as a product in FBP_A and as a modifier in RuBisCO, Starch_S).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{FBP} = v_5 - v_6 \tag{77}$$

8.7 Species F6P

Name F6P

Initial concentration $0.640764257004719\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in five reactions (as a reactant in F6P_TK, PG_I and as a product in FBPase and as a modifier in FBPase, Starch_S).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{F6P} = v_6 - v_7 - v_{14} \tag{78}$$

8.8 Species E4P

Name E4P

Initial concentration $0.05\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in SBP_A and as a product in F6P_TK).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{E4P} = v_7 - v_8 \tag{79}$$

8.9 Species SBP

Name SBP

Initial concentration $0.3\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in three reactions (as a reactant in SBPase and as a product in SBP_A and as a modifier in RuBisCO).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{SBP} = v_8 - v_9 \tag{80}$$

8.10 Species S7P

Name S7P

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

This species takes part in two reactions (as a reactant in S7P_TK and as a product in SBPase).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{S7P} = v_9 - v_{10} \tag{81}$$

8.11 Species X5P

Name X5P

Initial concentration $0.0747384155455904\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in three reactions (as a reactant in Ru5P_E and as a product in F6P_TK, S7P_TK).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{X5P} = v_7 + v_{10} - v_{12} \tag{82}$$

8.12 Species R5P

Name R5P

Initial concentration $0.125186846038864\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in R5P_I and as a product in S7P_TK).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{R5P} = v_{10} - v_{11} \tag{83}$$

8.13 Species Ru5P

Name Ru5P

Initial concentration $0.0500747384155456\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in three reactions (as a reactant in Ru5P_K and as a product in R5P_I, Ru5P_E).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Ru5P} = v_{11} + v_{12} - v_{13} \tag{84}$$

8.14 Species G6P

Name G6P

Initial concentration $1.47375779111085\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in PG_M and as a product in PG_I).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{G6P} = v_{14} - v_{15} \tag{85}$$

8.15 Species G1P

Name G1P

Initial concentration $0.0854779518844294\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in four reactions (as a reactant in Starch_S and as a product in PG_M, Starch_P and as a modifier in Starch_P).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{G1P} = v_{15} + v_{17} - v_{16} \tag{86}$$

8.16 Species ATP

Name ATP

Initial concentration $0.68\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in four reactions (as a reactant in PGA_K, Ru5P_K, Starch_S and as a product in ATP_S).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ATP} = v_{18} - v_{2} - v_{13} - v_{16} \tag{87}$$

8.17 Species ADP

Name ADP

Initial concentration $0.82\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

Involved in rule ADP

This species takes part in five reactions (as a reactant in ATP_S and as a product in PGA_K, Ru5P_K and as a modifier in Ru5P_K, Starch_S). Not these but one rule determines the species' quantity because this species is on the boundary of the reaction system.

8.18 Species NADPH

Name NADPH

Initial concentration $0.21\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in GAP_DH and as a modifier in RuBisCO), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{NADPH} = 0 \tag{88}$$

8.19 Species NADP

Name NADP

Initial concentration $0.29\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{NADP} = 0 \tag{89}$$

8.20 Species H

Name H

Initial concentration $1.25892541179417\cdot 10^{-5}\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{H} = 0 \tag{90}$$

8.21 Species Pi

Name Pi

Initial concentration $0.977800000000002\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

Involved in rule Pi

This species takes part in 13 reactions (as a reactant in Starch_P, ATP_S and as a product in GAP_DH, FBPase, SBPase and as a modifier in RuBisCO, FBPase, SBPase, Ru5P_K, Starch_S, TPT_PGA, TPT_GAP, TPT_DHAP). Not these but one rule determines the species' quantity because this species is on the boundary of the reaction system.

8.22 Species Pext

Name Pext

Initial concentration $0.5\ \mathrm{mmol} \cdot \mathrm{l}^{-1}$

This species takes part in three reactions (as a modifier in TPT_PGA, TPT_GAP, TPT_DHAP), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Pext} = 0 \tag{91}$$

A Glossary of Systems Biology Ontology Terms

SBO:0000009 kinetic constant: Numerical parameter that quantifies the velocity of a chemical reaction

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

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