# **SBML Model Report**

# Model name: "Arnold2011\_Hahn1986-\_CalvinCycle\_Starch\_Sucrose"



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<sup>1</sup>, Anne Arnold<sup>2</sup> and Zoran Nikoloski<sup>3</sup> at October 19<sup>th</sup> 2011 at 2:53 p.m. and last time modified at April 20<sup>th</sup> 2012 at 7:51 p.m. Table 1 gives an overview of the quantities of all components of this model.

Table 1: Number of components in this model, which are described in the following sections.

Element	Quantity	Element	Quantity
compartment types	0	compartments	4
species types	0	species	22
events	0	constraints	0
reactions	18	function definitions	1
global parameters	4	unit definitions	2
rules	1	initial assignments	0

#### **Model Notes**

This model is from the article:

# A quantitative comparison of CalvinBenson cycle models

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Anne Arnold, Zoran Nikoloski <u>Trends in Plant Science</u> 2011 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 pathways to starch and sucrose synthesis by Hahn (1986, [click here for abstract]). The parameter values are taken from Hahn (1984, [click here for abstract]). 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** ml

### 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<sup>2</sup>

### 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 four compartments.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
chloroplast	chloroplast		3	1	litre	$ \overline{\mathbf{Z}} $	
cytosol	cytosol		3	1	litre	$\overline{\mathbf{Z}}$	
vacuole	vacuole		3	1	litre	$   \overline{\mathbf{Z}} $	
phloem	phloem		3	1	litre	$   \overline{\mathbf{Z}} $	

# 3.1 Compartment chloroplast

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

Name chloroplast

# 3.2 Compartment cytosol

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

Name cytosol

# 3.3 Compartment vacuole

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

Name vacuole

# 3.4 Compartment phloem

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

Name phloem

# 4 Species

This model contains 22 species. The boundary condition of three of these species is set to true so that these species' amount cannot be changed by any reaction. Section 9 provides further details and the derived rates of change of each species.

Table 3: Properties of each species.

Id	Name	Compartment	Derived Unit	Constant	Boundary Condi- tion
RuBP	RuBP	chloroplast	$\mathrm{mmol}\cdot\mathrm{ml}^{-1}$		
PGA	PGA	chloroplast	$\mathrm{mmol}\cdot\mathrm{ml}^{-1}$	$\Box$	
TP	TP	chloroplast	$\mathrm{mmol}\cdot\mathrm{ml}^{-1}$	$\Box$	
HeP	HeP	chloroplast	$\mathrm{mmol}\cdot\mathrm{ml}^{-1}$	$\Box$	
TPGA	TPGA	chloroplast	$\mathrm{mmol}\cdot\mathrm{ml}^{-1}$	$\Box$	
E4P	E4P	chloroplast	$\mathrm{mmol}\cdot\mathrm{ml}^{-1}$	$\Box$	
S7P	S7P	chloroplast	$\mathrm{mmol}\cdot\mathrm{ml}^{-1}$	$\Box$	
Ru5P	Ru5P	chloroplast	$\mathrm{mmol}\cdot\mathrm{ml}^{-1}$	$\Box$	
GG	GG	chloroplast	$\mathrm{mmol}\cdot\mathrm{ml}^{-1}$	$\Box$	
ATP	ATP	chloroplast	$\mathrm{mmol}\cdot\mathrm{ml}^{-1}$		
ADP	ADP	chloroplast	$\mathrm{mmol}\cdot\mathrm{ml}^{-1}$	$\Box$	
UTP	UTP	chloroplast	$\mathrm{mmol}\cdot\mathrm{ml}^{-1}$	$\Box$	
UDP	UDP	chloroplast	$\mathrm{mmol}\cdot\mathrm{ml}^{-1}$	$\Box$	
Pi	Pi	chloroplast	$\mathrm{mmol}\cdot\mathrm{ml}^{-1}$	$\Box$	
C02	CO2	chloroplast	$\mathrm{mmol}\cdot\mathrm{ml}^{-1}$		$\square$
TPc	TPc	cytosol	$\mathrm{mmol}\cdot\mathrm{ml}^{-1}$		
HePc	HePc	cytosol	$\mathrm{mmol}\cdot\mathrm{ml}^{-1}$	$\Box$	
Suc	Suc	cytosol	$\mathrm{mmol}\cdot\mathrm{ml}^{-1}$	$\Box$	
Pic	Pic	cytosol	$\mathrm{mmol}\cdot\mathrm{ml}^{-1}$	$\Box$	
SucV	SucV	vacuole	$\mathrm{mmol}\cdot\mathrm{ml}^{-1}$	$\Box$	
E	Е	phloem	$\text{mmol}\cdot\text{ml}^{-1}$		

Id	Name	Compartment	Derived Unit	Constant	Boundary Condi- tion
Resp	Resp	chloroplast	$\mathrm{mmol}\cdot\mathrm{ml}^{-1}$		$ \overline{\checkmark} $

# **5 Parameters**

This model contains four global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
r	r	0000009	$3 \cdot 10^{-5}$		$\overline{Z}$
D	D	0000009	$10^{-4}$		$\overline{\mathbf{Z}}$
phi	phi	0000009	$10^{-4}$		
$v_{-}15$	v(15)	0000009	0.010		

# **6 Function definition**

This is an overview of one function definition.

# **6.1 Function definition** function\_1

Name irreversible Constant flux (Suc synth)

Argument v

**Mathematical Expression** 

v (1)

# 7 Rule

This is an overview of one rule.

### **7.1 Rule v\_15**

Rule v\_15 is an assignment rule for parameter v\_15:

$$v_{-}15 = 0.0258 \cdot [HePc] \cdot [UTP] \tag{2}$$

# 8 Reactions

This model contains 18 reactions. All reactions are listed in the following table and are subsequently described in detail. If a reaction is affected by a modifier, the identifier of this species is written above the reaction arrow.

Table 5: Overview of all reactions

N⁰	Id	Name	Reaction Equation	SBO
1	RuBisCO	RuBisCO	$RuBP + CO2 \longrightarrow 2PGA$	
2	PGA_red	PGA reduction	$PGA + ATP \longrightarrow TP + ADP + Pi$	
3	FBP_A_ase	FBP ald + ase	$2 \text{ TP} \Longrightarrow \text{HeP} + \text{Pi}$	
4	F6P_TK1	F6P trans I	$HeP \longrightarrow TPGA + E4P$	
5	$SBP\_A\_ase$	SBP ald + ase	$E4P + TP \longrightarrow S7P + Pi$	
6	S7P_TK1_R5P_I	S7P trans I + R5P iso	$S7P \longrightarrow TPGA + Ru5P$	
7	TK2_Ru5P_E	trans II + Ru5P epi	$TPGA + TP \longrightarrow Ru5P$	
8	Ru5P_K	Ru5P kinase	$Ru5P + ATP \longrightarrow RuBP + ADP$	
9	$ATP_S$	ATP synthase	$ADP + Pi \longrightarrow ATP$	
10	$Starch_S$	starch synthetase	$ATP + HeP \longrightarrow GG + ADP + 2Pi$	
11	$Starch\_P$	starch phosphorylase	$GG + Pi \longrightarrow HeP$	
12	TPT	TP translocator	$TP + Pic \longrightarrow TPc + Pi$	
13	FBPc_A_ase	FBPc ald + ase	$2  \text{TPc} \longrightarrow \text{HePc} + \text{Pic}$	
14	Suc_S	sucrose synthetase	$2 \text{ HePc} + \text{UTP} \longrightarrow \text{Suc} + \text{UDP} + 3 \text{ Pic}$	
15	UTP_S	UTP synthase	$UDP + Pic \longrightarrow UTP$	
16	Respi	respiration rate	$Suc \longrightarrow Resp$	
17	Diffu	diffusion rate	$Suc \Longrightarrow SucV$	
18	Transl	translocation rate	$Suc \rightleftharpoons E$	

### 8.1 Reaction RuBisCO

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

Name RuBisCO

# **Reaction equation**

$$RuBP + CO2 \longrightarrow 2PGA \tag{3}$$

### **Reactants**

Table 6: Properties of each reactant.

Id	Name	SBO
RuBP	RuBP	
C02	CO2	

# **Product**

Table 7: Properties of each product.

Id	Name	SBO
PGA	PGA	

#### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_1 = \text{vol}\left(\text{chloroplast}\right) \cdot \text{k1} \cdot [\text{RuBP}] \cdot [\text{CO2}]$$
 (4)

Table 8: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1	0000009	0.006		Ø

# 8.2 Reaction PGA\_red

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

Name PGA reduction

# **Reaction equation**

$$PGA + ATP \longrightarrow TP + ADP + Pi$$
 (5)

### **Reactants**

Table 9: Properties of each reactant.

Id	Name	SBO
PGA	PGA	
ATP	ATP	

#### **Products**

Table 10: Properties of each product.

Name	SBO
TP	
ADP	
Pi	
	TP ADP

### **Kinetic Law**

Derived unit contains undeclared units

$$v_2 = \text{vol}(\text{chloroplast}) \cdot \text{k1} \cdot [\text{PGA}] \cdot [\text{ATP}]$$
 (6)

Table 11: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1	0000009	0.021		Ø

### 8.3 Reaction FBP\_A\_ase

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

Name FBP ald + ase

# **Reaction equation**

$$2TP \Longrightarrow HeP + Pi \tag{7}$$

### Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
TP	TP	

# **Products**

Table 13: Properties of each product.

Id	Name	SBO
HeP	HeP	
Pi	Pi	

### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_3 = \text{vol}\left(\text{chloroplast}\right) \cdot \left(\text{k1} \cdot [\text{TP}]^2 - \text{k2} \cdot [\text{HeP}] \cdot [\text{Pi}]\right)$$
 (8)

Table 14: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1	0000009	4.0		$\square$
k2	k2	0000009	0.0		$\square$

### 8.4 Reaction F6P\_TK1

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

Name F6P trans I

# **Reaction equation**

$$HeP \longrightarrow TPGA + E4P$$
 (9)

# Reactant

Table 15: Properties of each reactant.

Id	Name	SBO
HeP	HeP	

### **Products**

Table 16: Properties of each product.

Id	Name	SBO
TPGA	TPGA	
E4P	E4P	

### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_4 = \text{vol}(\text{chloroplast}) \cdot \text{k1} \cdot [\text{HeP}]$$
 (10)

Table 17: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1	0000009	0.031		

### 8.5 Reaction SBP\_A\_ase

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

Name SBP ald + ase

# **Reaction equation**

$$E4P + TP \longrightarrow S7P + Pi \tag{11}$$

#### **Reactants**

Table 18: Properties of each reactant.

Id	Name	SBO
E4P	E4P	
TP	TP	

### **Products**

Table 19: Properties of each product.

Id	Name	SBO
S7P	S7P	
Pi	Pi	

#### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_5 = \text{vol}\left(\text{chloroplast}\right) \cdot \text{k1} \cdot [\text{E4P}] \cdot [\text{TP}]$$
 (12)

Table 20: Properties of each parameter.

Id	Name	SBO Value	Unit	Constant
k1	k1	0000009 3.1		

# 8.6 Reaction S7P\_TK1\_R5P\_I

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

Name S7P trans I + R5P iso

# **Reaction equation**

$$S7P \longrightarrow TPGA + Ru5P \tag{13}$$

### Reactant

Table 21: Properties of each reactant.

Id	Name	SBO
S7P	S7P	

# **Products**

Table 22: Properties of each product.

Id	Name	SBO
TPGA	TPGA	
Ru5P	Ru5P	

# **Kinetic Law**

**Derived unit** contains undeclared units

$$v_6 = \text{vol}\left(\text{chloroplast}\right) \cdot \text{k1} \cdot [\text{S7P}]$$
 (14)

Table 23: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	<b>k</b> 1	0000009 0.31	

# 8.7 Reaction TK2\_Ru5P\_E

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

Name trans II + Ru5P epi

# **Reaction equation**

$$TPGA + TP \longrightarrow Ru5P \tag{15}$$

### Reactants

Table 24: Properties of each reactant.

Id	Name	SBO
TPGA	TPGA	
TP	TP	

### **Product**

Table 25: Properties of each product.

Id	Name	SBO
Ru5P	Ru5P	

### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_7 = \text{vol}(\text{chloroplast}) \cdot \text{k1} \cdot [\text{TPGA}] \cdot [\text{TP}]$$
 (16)

Table 26: Properties of each parameter.

Id	Name	SBO Value	Unit	Constant
k1	k1	0000009 6.2		$\square$

### 8.8 Reaction Ru5P\_K

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

Name Ru5P kinase

### **Reaction equation**

$$Ru5P + ATP \longrightarrow RuBP + ADP \tag{17}$$

#### **Reactants**

Table 27: Properties of each reactant.

P

### **Products**

Table 28: Properties of each product.

Id	Name	SBO
RuBP ADP	RuBP ADP	

#### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_8 = \text{vol}\left(\text{chloroplast}\right) \cdot \text{k1} \cdot [\text{Ru5P}] \cdot [\text{ATP}]$$
 (18)

Table 29: Properties of each parameter.

Id	Name	SBO	Value U	Unit	Constant
k1	k1	0000009	0.031		

### 8.9 Reaction ATP\_S

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

Name ATP synthase

# **Reaction equation**

$$ADP + Pi \longrightarrow ATP \tag{19}$$

#### **Reactants**

Table 30: Properties of each reactant.

Id	Name	SBO
ADP	ADP	
Pi	Pi	

### **Product**

Table 31: Properties of each product.

Id	Name	SBO
ATP	ATP	

#### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_9 = \text{vol}\left(\text{chloroplast}\right) \cdot \text{k1} \cdot [\text{ADP}] \cdot [\text{Pi}]$$
 (20)

Table 32: Properties of each parameter.

Id	Name	SBO V	Value	Unit	Constant
k1	k1	0000009	0.279		

### 8.10 Reaction Starch\_S

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

Name starch synthetase

# **Reaction equation**

$$ATP + HeP \longrightarrow GG + ADP + 2Pi$$
 (21)

### **Reactants**

Table 33: Properties of each reactant.

Id	Name	SBO
ATP	ATP	
HeP	HeP	

### **Products**

Table 34: Properties of each product.

Name	SBO
GG	_
ADP	
Pi	
	GG ADP

#### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{10} = \text{vol}\left(\text{chloroplast}\right) \cdot \text{k1} \cdot [\text{ATP}] \cdot [\text{HeP}]$$
 (22)

Table 35: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1	0000009	0.002		Ø

# 8.11 Reaction Starch\_P

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

Name starch phosphorylase

# **Reaction equation**

$$GG + Pi \longrightarrow HeP$$
 (23)

### **Reactants**

Table 36: Properties of each reactant.

Id	Name	SBO
GG	GG	
Pi	Pi	

### **Product**

Table 37: Properties of each product.

Id	Name	SBO
HeP	HeP	

### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{11} = vol\left(chloroplast\right) \cdot k1 \cdot [GG] \cdot [Pi] \tag{24}$$

Table 38: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	k1	$0000009  4 \cdot 10^{-5}$	$\overline{Z}$

# 8.12 Reaction TPT

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

Name TP translocator

# **Reaction equation**

$$TP + Pic \longrightarrow TPc + Pi$$
 (25)

### **Reactants**

Table 39: Properties of each reactant.

Id	Name	SBO
TP	TP	
Pic	Pic	

#### **Products**

Table 40: Properties of each product.

Id	Name	SBO
TPc	TPc	
Pi	Pi	

### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{12} = k1 \cdot [TP] \cdot [Pic] \tag{26}$$

Table 41: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1	0000009	0.5		

# 8.13 Reaction FBPc\_A\_ase

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

Name FBPc ald + ase

# **Reaction equation**

$$2 \, \text{TPc} \longrightarrow \text{HePc} + \text{Pic} \tag{27}$$

# Reactant

Table 42: Properties of each reactant.

Id	Name	SBO
TPc	TPc	

### **Products**

Table 43: Properties of each product.

Id	Name	SBO
НеРс	HePc	
Pic	Pic	

### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{13} = \text{vol}(\text{cytosol}) \cdot \text{k1} \cdot [\text{TPc}]^2$$
 (28)

Table 44: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1	0000009	1.55		$\overline{Z}$

### 8.14 Reaction Suc\_S

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

Name sucrose synthetase

### **Reaction equation**

$$2 \text{HePc} + \text{UTP} \longrightarrow \text{Suc} + \text{UDP} + 3 \text{Pic}$$
 (29)

# **Reactants**

Table 45: Properties of each reactant.

Id	Name	SBO
HePc	HePc	
UTP	UTP	

### **Products**

Table 46: Properties of each product.

Id	Name	SBO
Suc	Suc	
UDP	UDP	
Pic	Pic	

# **Kinetic Law**

**Derived unit** not available

$$v_{14} = \text{function}_{-1} (v_{-15})$$
 (30)

$$function_{-}1(v) = v (31)$$

# 8.15 Reaction UTP\_S

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

Name UTP synthase

# **Reaction equation**

$$UDP + Pic \longrightarrow UTP \tag{32}$$

### **Reactants**

Table 47: Properties of each reactant.

Id	Name	SBO
UDP	UDP	
Pic	Pic	

#### **Product**

Table 48: Properties of each product.

Id	Name	SBO
UTP	UTP	

### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{15} = k1 \cdot [UDP] \cdot [Pic] \tag{33}$$

Table 49: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1	0000009	0.008		

# 8.16 Reaction Respi

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

Name respiration rate

# **Reaction equation**

$$Suc \longrightarrow Resp \tag{34}$$

#### Reactant

Table 50: Properties of each reactant.

Id	Name	SBO
Suc	Suc	

### **Product**

Table 51: Properties of each product.

Id	Name	SBO
Resp	Resp	

#### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{16} = r \cdot [Suc] \tag{35}$$

### 8.17 Reaction Diffu

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

Name diffusion rate

# **Reaction equation**

$$Suc \rightleftharpoons SucV$$
 (36)

### Reactant

Table 52: Properties of each reactant.

Id	Name	SBO
Suc	Suc	

### **Product**

Table 53: Properties of each product.

Id	Name	SBO
SucV	SucV	

# **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{17} = D \cdot [Suc] - D \cdot [SucV]$$
(37)

# 8.18 Reaction Transl

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

Name translocation rate

# **Reaction equation**

$$Suc \rightleftharpoons E$$
 (38)

### Reactant

Table 54: Properties of each reactant.

Id	Name	SBO
Suc	Suc	

#### **Product**

Table 55: Properties of each product.

Id	Name	SBO
E	E	

#### **Kinetic Law**

**Derived unit** contains undeclared units

$$v_{18} = \text{phi} \cdot [\text{Suc}] - \text{phi} \cdot [\text{E}] \tag{39}$$

# 9 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.

# 9.1 Species RuBP

Name RuBP

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

This species takes part in two reactions (as a reactant in RuBisCO and as a product in Ru5P\_K).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{RuBP} = |v_8| - |v_1| \tag{40}$$

# 9.2 Species PGA

Name PGA

Initial concentration 2.4 mmol⋅ml<sup>-1</sup>

This species takes part in two reactions (as a reactant in PGA\_red and as a product in RuBisCO).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{PGA} = 2 v_1 - v_2 \tag{41}$$

### 9.3 Species TP

Name TP

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

This species takes part in five reactions (as a reactant in FBP\_A\_ase, SBP\_A\_ase, TK2\_Ru5P\_E, TPT and as a product in PGA\_red).

$$\frac{d}{dt}TP = |v_2| - 2|v_3| - |v_5| - |v_7| - |v_{12}|$$
(42)

### 9.4 Species HeP

Name HeP

Initial concentration  $2.2 \text{ mmol} \cdot \text{ml}^{-1}$ 

This species takes part in four reactions (as a reactant in F6P\_TK1, Starch\_S and as a product in FBP\_A\_ase, Starch\_P).

$$\frac{d}{dt}HeP = |v_3| + |v_{11}| - |v_4| - |v_{10}|$$
(43)

#### 9.5 Species TPGA

Name TPGA

Notes TPGA = R5P + X5P

Initial concentration  $0.2 \text{ } \text{mmol} \cdot \text{ml}^{-1}$ 

This species takes part in three reactions (as a reactant in TK2\_Ru5P\_E and as a product in F6P-TK1, S7P\_TK1\_R5P\_I).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{TPGA} = |v_4| + |v_6| - |v_7| \tag{44}$$

### 9.6 Species E4P

Name E4P

Initial concentration  $0.05 \text{ } \text{mmol} \cdot \text{ml}^{-1}$ 

This species takes part in two reactions (as a reactant in SBP\_A\_ase and as a product in F6P\_TK1).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{E}4\mathrm{P} = |v_4| - |v_5| \tag{45}$$

### 9.7 Species S7P

Name S7P

Initial concentration 2 mmol·ml<sup>-1</sup>

This species takes part in two reactions (as a reactant in S7P\_TK1\_R5P\_I and as a product in SBP\_A\_ase).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{S7P} = v_5 - v_6 \tag{46}$$

### 9.8 Species Ru5P

Name Ru5P

Initial concentration  $0.05~\text{mmol}\cdot\text{ml}^{-1}$ 

This species takes part in three reactions (as a reactant in Ru5P\_K and as a product in S7P\_TK1-\_R5P\_I, TK2\_Ru5P\_E).

$$\frac{d}{dt}Ru5P = v_6 + v_7 - v_8 \tag{47}$$

# 9.9 Species GG

Name GG

Notes Hahn et al. (1984) Table 1

This species takes part in two reactions (as a reactant in Starch\_P and as a product in Starch\_S).

$$\frac{\mathrm{d}}{\mathrm{d}t}GG = |v_{10}| - |v_{11}| \tag{48}$$

# 9.10 Species ATP

Name ATP

Notes Hahn et al. (1984) Table 1

Initial concentration 3.875 mmol⋅ml<sup>-1</sup>

This species takes part in four reactions (as a reactant in PGA\_red, Ru5P\_K, Starch\_S and as a product in ATP\_S).

$$\frac{d}{dt}ATP = |v_9| - |v_2| - |v_8| - |v_{10}| \tag{49}$$

### 9.11 Species ADP

Name ADP

Notes Hahn et al. (1984) Table 1

Initial concentration  $0.53 \text{ } \text{mmol} \cdot \text{ml}^{-1}$ 

This species takes part in four reactions (as a reactant in ATP\_S and as a product in PGA\_red, Ru5P\_K, Starch\_S).

$$\frac{d}{dt}ADP = |v_2| + |v_8| + |v_{10}| - |v_9|$$
 (50)

# 9.12 Species UTP

Name UTP

Notes Hahn et al. (1984) Table 1

Initial concentration  $3.871 \text{ mmol} \cdot \text{ml}^{-1}$ 

This species takes part in two reactions (as a reactant in Suc\_S and as a product in UTP\_S).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{UTP} = |v_{15}| - |v_{14}| \tag{51}$$

### 9.13 Species UDP

Name UDP

Notes Hahn et al. (1984) Table 1

Initial concentration  $1.613 \text{ mmol} \cdot \text{ml}^{-1}$ 

This species takes part in two reactions (as a reactant in UTP\_S and as a product in Suc\_S).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{UDP} = |v_{14}| - |v_{15}| \tag{52}$$

# 9.14 Species Pi

Name Pi

Notes Hahn et al. (1984) Table 1

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

This species takes part in seven reactions (as a reactant in ATP\_S, Starch\_P and as a product in PGA\_red, FBP\_A\_ase, SBP\_A\_ase, Starch\_S, TPT).

$$\frac{\mathrm{d}}{\mathrm{d}t} \mathrm{Pi} = |v_2| + |v_3| + |v_5| + 2|v_{10}| + |v_{12}| - |v_9| - |v_{11}| \tag{53}$$

### **9.15 Species** C02

Name CO2

Notes [Pa] Hahn et al. (1984) Table 2

Initial concentration  $31 \text{ mmol} \cdot \text{ml}^{-1}$ 

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{CO2} = 0\tag{54}$$

# 9.16 Species TPc

Name TPc

Notes Hahn et al. (1984) Table 1

Initial concentration  $0.114 \text{ mmol} \cdot \text{ml}^{-1}$ 

This species takes part in two reactions (as a reactant in FBPc\_A\_ase and as a product in TPT).

$$\frac{d}{dt}TPc = v_{12} - 2v_{13} \tag{55}$$

### 9.17 Species HePc

Name HePc

Notes Hahn et al. (1984) Table 1

Initial concentration  $0.1 \text{ mmol} \cdot \text{ml}^{-1}$ 

This species takes part in two reactions (as a reactant in Suc\_S and as a product in FBPc\_A\_ase).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{HePc} = v_{13} - 2 v_{14} \tag{56}$$

### 9.18 Species Suc

Name Suc

Notes Hahn et al. (1984) Table 1

Initial concentration 77.31 mmol⋅ml<sup>-1</sup>

This species takes part in four reactions (as a reactant in Respi, Diffu, Transl and as a product in Suc\_S).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Suc} = |v_{14}| - |v_{16}| - |v_{17}| - |v_{18}| \tag{57}$$

### 9.19 Species Pic

Name Pic

Notes Hahn et al. (1984) Table 1

Initial concentration  $0.8 \text{ } \text{mmol} \cdot \text{ml}^{-1}$ 

This species takes part in four reactions (as a reactant in TPT, UTP\_S and as a product in FBPc-\_A\_ase, Suc\_S).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Pic} = v_{13} + 3 v_{14} - v_{12} - v_{15} \tag{58}$$

### 9.20 Species SucV

Name SucV

Notes Hahn et al. (1984) Table 1

Initial concentration 77.31 mmol⋅ml<sup>-1</sup>

This species takes part in one reaction (as a product in Diffu).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{SucV} = v_{17} \tag{59}$$

### 9.21 Species E

Name E

SBO:0000009 kinetic constant

Notes Hahn et al. (1984) Table 2

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

This species takes part in one reaction (as a product in Trans1), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

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

# 9.22 Species Resp

Name Resp

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

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

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

# A Glossary of Systems Biology Ontology Terms

**SBO:000009 kinetic constant:** Numerical parameter that quantifies the velocity of a chemical reaction

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