

SBML Model Report

Model name: “Poolman2004_CalvinCycle”



May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 1 format. This model was created by the following four authors: Nicolas Le Novre¹, Herbert Sauro², Mark Poolman³ and Lukas Endler⁴ at June 25th 2008 at 3:14 p. m. and last time modified at February 25th 2015 at 12:23 a. 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	27
events	0	constraints	0
reactions	21	function definitions	0
global parameters	1	unit definitions	1
rules	0	initial assignments	0

Model Notes

This a model from the article:

Applications of metabolic modelling to plant metabolism.

Poolman MG ,Assmus HE, Fell DA J. Exp. Bot.[2004 May; Volume: 55 (Issue: 400)]: 1177-86
[15073223](#),

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Abstract:

In this paper some of the general concepts underpinning the computer modelling of metabolic systems are introduced. The difference between kinetic and structural modelling is emphasized, and the more important techniques from both, along with the physiological implications, are described. These approaches are then illustrated by descriptions of other work, in which they have been applied to models of the Calvin cycle, sucrose metabolism in sugar cane, and starch metabolism in potatoes.

This model describes the non oxidative Calvin cycle as depicted in Poolman et al; J Exp Bot (2004) 55:1177-1186, fig 2. Reaction E20: $E4P + F6P \rightleftharpoons S7P + GAP$, is depicted in the figure, but not included in the model. The light reaction: $ADP + P_i \rightarrow ATP$, is included in the model, but only mentioned in the figure caption. The parameters and initial concentrations are the same as in Poolman, 1999, Computer Modelling Applied to the Calvin Cycle, PhD Thesis, Oxford Brookes University, Appendix A (available at <http://mudshark.brookes.ac.uk/index.php/Publications/Theses/Mark>)

Mark Poolman (mgpoolman@brookes.ac.uk) 1995-2002

Based on a description by Pettersson 1988, Eur. J. Biochem. 175, 661-672

Differences are:

- 1 - Reactions assumed by Pettersson to be in equilibrium have fast mass action kinetics.
- 2 - Introduction of the parameter PGXpMult to modulate PGA export through TPT.
- 3 - Introduction of Starch phosphorylase reaction.

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- 1 - This notice is reproduced in its entirety
- 2 - Published material making use of (information gained from) this model cites at least:
 - (a) Poolman, 1999, Computer Modelling Applied to the Calvin Cycle, PhD Thesis, Oxford Brookes University
 - (b) Poolman, Fell, and Thomas. 2000, Modelling Photosynthesis and its control, J. Exp. Bot. 51, 319-328

or

- (c) Poolman et al. 2001, Computer modelling and experimental evidence for two steady states in the photosynthetic Calvin cycle. Eur. J. Biochem. 268, 2810-2816

Further related information may be found at <http://mudshark.brookes.ac.uk>.

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To cite BioModels Database, please use: Li C, Donizelli M, Rodriguez N, Dharuri H, Endler L, Chelliah V, Li L, He E, Henry A, Stefan MI, Snoep JL, Hucka M, Le Novre N, Laibe C (2010) BioModels Database: An enhanced, curated and annotated resource for published quantitative kinetic models. BMC Syst Biol., 4:92.

2 Unit Definitions

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

2.1 Unit substance

Name mM

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 m²

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			3	1	litre	<input checked="" type="checkbox"/>	
cytosol			3	1	litre	<input checked="" type="checkbox"/>	

3.1 Compartment `chloroplast`

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

3.2 Compartment `cytosol`

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

4 Species

This model contains 27 species. The boundary condition of nine of these species is set to `true` so that these species' amount cannot be changed by any reaction. 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
x_CO2		chloroplast	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input checked="" type="checkbox"/>
RuBP_ch		chloroplast	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
PGA_ch		chloroplast	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
ATP_ch		chloroplast	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
BPGA_ch		chloroplast	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
x_NADPH_ch		chloroplast	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input checked="" type="checkbox"/>
GAP_ch		chloroplast	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
Pi_ch		chloroplast	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
DHAP_ch		chloroplast	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
FBP_ch		chloroplast	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
F6P_ch		chloroplast	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
E4P_ch		chloroplast	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
X5P_ch		chloroplast	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
SBP_ch		chloroplast	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
S7P_ch		chloroplast	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
R5P_ch		chloroplast	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
Ru5P_ch		chloroplast	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
x_Pi_cyt		cytosol	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input checked="" type="checkbox"/>
x_GAP_cyt		cytosol	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input checked="" type="checkbox"/>
G6P_ch		chloroplast	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
x_NADP_ch		chloroplast	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input checked="" type="checkbox"/>

Id	Name	Compartment	Derived Unit	Constant	Boundary Condi- tion
x_PGA_cyt		cytosol	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input checked="" type="checkbox"/>
ADP_ch		chloroplast	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
x_DHAP_cyt		cytosol	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input checked="" type="checkbox"/>
x_Proton_ch		chloroplast	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input checked="" type="checkbox"/>
G1P_ch		chloroplast	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
x_Starch_ch		chloroplast	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input checked="" type="checkbox"/>

5 Parameter

This model contains one global parameter.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Light_on			1.0		<input checked="" type="checkbox"/>

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 5: Overview of all reactions

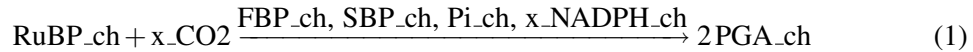
Nº	Id	Name	Reaction Equation	SBO
1	E1		$\text{RuBP_ch} + x_CO2 \xrightarrow{\text{FBP_ch, SBP_ch, Pi_ch, x_NADPH_ch}} 2 \text{PGA_ch}$	
2	E2		$\text{PGA_ch} + \text{ATP_ch} \longrightarrow \text{BPGA_ch} + \text{ADP_ch}$	
3	E3		$x_NADPH_ch + \text{BPGA_ch} + x_Proton_ch \longrightarrow x_NADP_ch + \text{GAP_ch} + \text{Pi_ch}$	
4	E4		$\text{GAP_ch} \rightleftharpoons \text{DHAP_ch}$	
5	E5		$\text{GAP_ch} + \text{DHAP_ch} \rightleftharpoons \text{FBP_ch}$	
6	E6		$\text{FBP_ch} \longrightarrow \text{F6P_ch} + \text{Pi_ch}$	
7	E7		$\text{GAP_ch} + \text{F6P_ch} \rightleftharpoons \text{X5P_ch} + \text{E4P_ch}$	
8	E8		$\text{DHAP_ch} + \text{E4P_ch} \rightleftharpoons \text{SBP_ch}$	
9	E9		$\text{SBP_ch} \longrightarrow \text{Pi_ch} + \text{S7P_ch}$	
10	E10		$\text{S7P_ch} + \text{GAP_ch} \rightleftharpoons \text{R5P_ch} + \text{X5P_ch}$	
11	E11		$\text{R5P_ch} \rightleftharpoons \text{Ru5P_ch}$	
12	E12		$\text{X5P_ch} \rightleftharpoons \text{Ru5P_ch}$	
13	E13		$\text{Ru5P_ch} + \text{ATP_ch} \xrightarrow{\text{PGA_ch, Pi_ch}} \text{RuBP_ch} + \text{ADP_ch}$	
14	E14		$\text{F6P_ch} \rightleftharpoons \text{G6P_ch}$	
15	E15		$\text{G6P_ch} \rightleftharpoons \text{G1P_ch}$	
16	light_reaction		$\text{Pi_ch} + \text{ADP_ch} \longrightarrow \text{ATP_ch}$	
17	E16		$\text{ATP_ch} + \text{G1P_ch} \xrightarrow{\text{PGA_ch, F6P_ch, FBP_ch}} x_Starch_ch + \text{ADP_ch} + 2 \text{Pi_ch}$	
18	E17		$x_Starch_ch + \text{Pi_ch} \longrightarrow \text{G1P_ch}$	

Nº	Id	Name	Reaction Equation	SBO
19	E18_DHAP		$x_Pi_cyt + DHAP_ch \xrightarrow{PGA_ch, GAP_ch} x_DHAP_cyt + Pi_ch$	
20	E18_PGA		$x_Pi_cyt + PGA_ch \xrightarrow{DHAP_ch, GAP_ch} x_PGA_cyt + Pi_ch$	
21	E18_GAP		$x_Pi_cyt + GAP_ch \xrightarrow{PGA_ch, DHAP_ch} x_GAP_cyt + Pi_ch$	

6.1 Reaction E1

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

Reaction equation



Reactants

Table 6: Properties of each reactant.

Id	Name	SBO
RuBP_ch		
x_CO2		

Modifiers

Table 7: Properties of each modifier.

Id	Name	SBO
FBP_ch		
SBP_ch		
Pi_ch		
x_NADPH_ch		

Product

Table 8: Properties of each product.

Id	Name	SBO
PGA_ch		

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \frac{\text{Light_on} \cdot \text{Rbco_vm} \cdot [\text{RuBP_ch}] \cdot \text{vol}(\text{chloroplast})}{[\text{RuBP_ch}] + \text{Rbco_km} \cdot \left(1 + \frac{[\text{PGA_ch}]}{\text{Rbco_KiPGA}} + \frac{[\text{FBP_ch}]}{\text{Rbco_KiFBP}} + \frac{[\text{SBP_ch}]}{\text{Rbco_KiSBP}} + \frac{[\text{Pi_ch}]}{\text{Rbco_KiPi}} + \frac{[\text{x_NADPH_ch}]}{\text{Rbco_KiNADPH}} \right)} \quad (2)$$

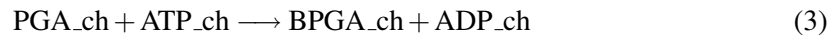
Table 9: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Rbco_vm			340.000		✓
Rbco_km			0.020		✓
Rbco_KiPGA			0.840		✓
Rbco_KiFBP			0.040		✓
Rbco_KiSBP			0.075		✓
Rbco_KiPi			0.900		✓
Rbco_KiNADPH			0.070		✓

6.2 Reaction E2

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

Reaction equation



Reactants

Table 10: Properties of each reactant.

Id	Name	SBO
	PGA_ch	
	ATP_ch	

Products

Table 11: Properties of each product.

Id	Name	SBO
	BPGA_ch	
	ADP_ch	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \text{Light_on} \cdot \text{PGK_v} \cdot \text{vol}(\text{chloroplast}) \cdot \left([\text{PGA_ch}] \cdot [\text{ATP_ch}] - \frac{[\text{BPGA_ch}] \cdot [\text{ADP_ch}]}{q_2} \right) \quad (4)$$

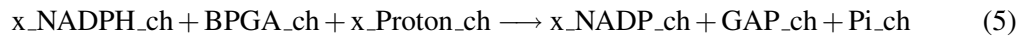
Table 12: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
PGK_v			$5 \cdot 10^8$		<input checked="" type="checkbox"/>
q2			$3.1 \cdot 10^{-4}$		<input checked="" type="checkbox"/>

6.3 Reaction E3

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

Reaction equation



Reactants

Table 13: Properties of each reactant.

Id	Name	SBO
x_NADPH_ch		
BPGA_ch		
x_Proton_ch		

Products

Table 14: Properties of each product.

Id	Name	SBO
x_NADP_ch		
GAP_ch		
Pi_ch		

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \text{Light_on} \cdot G3Pdh_v \cdot \text{vol}(\text{chloroplast}) \cdot \left([BPGA_ch] \cdot [x_NADPH_ch] \cdot [x_Proton_ch] - \frac{[x_NADP_ch] \cdot [GAP_ch] \cdot [Pi_ch]}{q3} \right) \quad (6)$$

Table 15: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
G3Pdh_v			$5 \cdot 10^8$		<input checked="" type="checkbox"/>
q3			$1.6 \cdot 10^7$		<input checked="" type="checkbox"/>

6.4 Reaction E4

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

Reaction equation



Reactant

Table 16: Properties of each reactant.

Id	Name	SBO
GAP_ch		

Product

Table 17: Properties of each product.

Id	Name	SBO
DHAP_ch		

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \text{vol}(\text{chloroplast}) \cdot \text{TPI_v} \cdot \left([\text{GAP_ch}] - \frac{[\text{DHAP_ch}]}{q_4} \right) \quad (8)$$

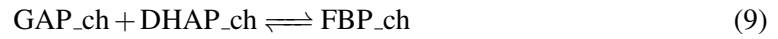
Table 18: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
TPI_v			$5 \cdot 10^8$		<input checked="" type="checkbox"/>
q4			22.000		<input checked="" type="checkbox"/>

6.5 Reaction E5

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

Reaction equation



Reactants

Table 19: Properties of each reactant.

Id	Name	SBO
GAP_ch		
DHAP_ch		

Product

Table 20: Properties of each product.

Id	Name	SBO
FBP_ch		

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \text{F_Aldo_v} \cdot \text{vol}(\text{chloroplast}) \cdot \left([\text{DHAP_ch}] \cdot [\text{GAP_ch}] - \frac{[\text{FBP_ch}]}{q_5} \right) \quad (10)$$

Table 21: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
F_Aldo_v			$5 \cdot 10^8$		<input checked="" type="checkbox"/>
q5			7.100		<input checked="" type="checkbox"/>

6.6 Reaction E6

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

Reaction equation



Reactant

Table 22: Properties of each reactant.

Id	Name	SBO
FBP_ch		

Products

Table 23: Properties of each product.

Id	Name	SBO
F6P_ch		
Pi_ch		

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \frac{\text{Light_on} \cdot \text{FBPase_ch_vm} \cdot [\text{FBP_ch}] \cdot \text{vol}(\text{chloroplast})}{[\text{FBP_ch}] + \text{FBPase_ch_km} \cdot \left(1 + \frac{[\text{F6P_ch}]}{\text{FBPase_ch_KiF6P}} + \frac{[\text{Pi_ch}]}{\text{FBPase_ch_KiPi}} \right)} \quad (12)$$

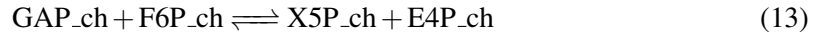
Table 24: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
FBPase_ch_vm			200.00		✓
FBPase_ch_km			0.03		✓
FBPase_ch- _KiF6P			0.70		✓
FBPase_ch- _KiPi			12.00		✓

6.7 Reaction E7

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

Reaction equation



Reactants

Table 25: Properties of each reactant.

Id	Name	SBO
GAP_ch		
F6P_ch		

Products

Table 26: Properties of each product.

Id	Name	SBO
X5P_ch		
E4P_ch		

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \text{vol}(\text{chloroplast}) \cdot F_{\text{TKL_v}} \cdot \left([\text{F6P_ch}] \cdot [\text{GAP_ch}] - \frac{[\text{E4P_ch}] \cdot [\text{X5P_ch}]}{q_7} \right) \quad (14)$$

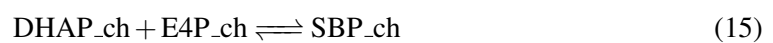
Table 27: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
F_TKL_v			$5 \cdot 10^8$		<input checked="" type="checkbox"/>
q7			0.084		<input checked="" type="checkbox"/>

6.8 Reaction E8

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

Reaction equation



Reactants

Table 28: Properties of each reactant.

Id	Name	SBO
	DHAP_ch	
	E4P_ch	

Product

Table 29: Properties of each product.

Id	Name	SBO
	SBP_ch	

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \text{vol}(\text{chloroplast}) \cdot E_{\text{Aldo}_v} \cdot \left([\text{E4P}_{\text{ch}}] \cdot [\text{DHAP}_{\text{ch}}] - \frac{[\text{SBP}_{\text{ch}}]}{q_8} \right) \quad (16)$$

Table 30: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
	E_Aldo_v		$5 \cdot 10^8$		<input checked="" type="checkbox"/>
	q8		13.000		<input checked="" type="checkbox"/>

6.9 Reaction E9

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

Reaction equation



Reactant

Table 31: Properties of each reactant.

Id	Name	SBO
SBP_ch		

Products

Table 32: Properties of each product.

Id	Name	SBO
Pi_ch		
S7P_ch		

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \frac{\text{Light_on} \cdot \text{SBPase_ch_vm} \cdot [\text{SBP_ch}] \cdot \text{vol}(\text{chloroplast})}{[\text{SBP_ch}] + \text{SBPase_ch_km} \cdot \left(1 + \frac{[\text{Pi_ch}]}{\text{SBPase_ch_KiPi}}\right)} \quad (18)$$

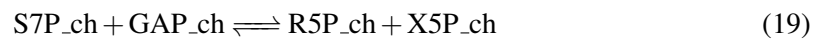
Table 33: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
SBPase_ch_vm			40.000		<input checked="" type="checkbox"/>
SBPase_ch_km			0.013		<input checked="" type="checkbox"/>
SBPase_ch_KiPi			12.000		<input checked="" type="checkbox"/>

6.10 Reaction E10

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

Reaction equation



Reactants

Table 34: Properties of each reactant.

Id	Name	SBO
S7P_ch		
GAP_ch		

Products

Table 35: Properties of each product.

Id	Name	SBO
R5P_ch		
X5P_ch		

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = \text{vol}(\text{chloroplast}) \cdot G_TKL_v \cdot \left([\text{GAP_ch}] \cdot [\text{S7P_ch}] - \frac{[\text{X5P_ch}] \cdot [\text{R5P_ch}]}{q_{10}} \right) \quad (20)$$

Table 36: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
G_TKL_v			$5 \cdot 10^8$		<input checked="" type="checkbox"/>
q10			0.850		<input checked="" type="checkbox"/>

6.11 Reaction E11

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

Reaction equation



Reactant

Table 37: Properties of each reactant.

Id	Name	SBO
R5P_ch		

Id	Name	SBO
----	------	-----

Product

Table 38: Properties of each product.

Id	Name	SBO
	Ru5P_ch	

Kinetic Law

Derived unit contains undeclared units

$$v_{11} = R5Piso_v \cdot \text{vol}(\text{chloroplast}) \cdot \left([R5P_ch] - \frac{[Ru5P_ch]}{q11} \right) \quad (22)$$

Table 39: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
	R5Piso_v		$5 \cdot 10^8$		<input checked="" type="checkbox"/>
	q11		0.400		<input checked="" type="checkbox"/>

6.12 Reaction E12

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

Reaction equation



Reactant

Table 40: Properties of each reactant.

Id	Name	SBO
	X5P_ch	

Product

Table 41: Properties of each product.

Id	Name	SBO
Ru5P_ch		

Kinetic Law

Derived unit contains undeclared units

$$v_{12} = \text{vol}(\text{chloroplast}) \cdot \text{X5Pepi_v} \cdot \left([\text{X5P_ch}] - \frac{[\text{Ru5P_ch}]}{q_{12}} \right) \quad (24)$$

Table 42: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
X5Pepi_v			$5 \cdot 10^8$		<input checked="" type="checkbox"/>
q12			0.670		<input checked="" type="checkbox"/>

6.13 Reaction E13

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

Reaction equation



Reactants

Table 43: Properties of each reactant.

Id	Name	SBO
Ru5P_ch		
ATP_ch		

Modifiers

Table 44: Properties of each modifier.

Id	Name	SBO
	PGA_ch	
	Pi_ch	

Products

Table 45: Properties of each product.

Id	Name	SBO
	RuBP_ch	
	ADP_ch	

Kinetic Law

Derived unit contains undeclared units

$$v_{13} = \frac{\text{Light_on} \cdot \text{Ru5Pk_ch_vm} \cdot [\text{Ru5P_ch}] \cdot \text{vol}(\text{chloroplast}) \cdot [\text{ATP_ch}]}{([\text{Ru5P_ch}] + \text{Ru5Pk_ch_km1} \cdot \left(1 + \frac{[\text{PGA_ch}]}{\text{Ru5Pk_ch_KiPGA}} + \frac{[\text{RuBP_ch}]}{\text{Ru5Pk_ch_KiRuBP}} + \frac{[\text{Pi_ch}]}{\text{Ru5Pk_ch_KiPi}}\right)) \cdot ([\text{ATP_ch}] \cdot \left(1 + \frac{[\text{ADP_ch}]}{\text{Ru5Pk_ch_KiADP1}} + \frac{[\text{ADP_ch}]}{\text{Ru5Pk_ch_KiADP2}}\right))} \quad (26)$$

Table 46: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
	Ru5Pk_ch_vm		10000.00		✓
	Ru5Pk_ch_km1		0.05		✓
	Ru5Pk_ch-_KiPGA		2.00		✓
	Ru5Pk_ch-_KiRuBP		0.70		✓
	Ru5Pk_ch-_KiPi		4.00		✓
	Ru5Pk_ch-_KiADP1		2.50		✓
	Ru5Pk_ch_km2		0.05		✓
	Ru5Pk_ch-_KiADP2		0.40		✓

6.14 Reaction E14

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

Reaction equation



Reactant

Table 47: Properties of each reactant.

Id	Name	SBO
F6P_ch		

Product

Table 48: Properties of each product.

Id	Name	SBO
G6P_ch		

Kinetic Law

Derived unit contains undeclared units

$$v_{14} = \text{PGI_v} \cdot \text{vol}(\text{chloroplast}) \cdot \left([\text{F6P_ch}] - \frac{[\text{G6P_ch}]}{q_{14}} \right) \quad (28)$$

Table 49: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
PGI_v			$5 \cdot 10^8$		<input checked="" type="checkbox"/>
q14			2.300		<input checked="" type="checkbox"/>

6.15 Reaction E15

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

Reaction equation



Reactant

Table 50: Properties of each reactant.

Id	Name	SBO
G6P_ch		

Product

Table 51: Properties of each product.

Id	Name	SBO
G1P_ch		

Kinetic Law

Derived unit contains undeclared units

$$v_{15} = \text{PGM_v} \cdot \text{vol}(\text{chloroplast}) \cdot \left([\text{G6P_ch}] - \frac{[\text{G1P_ch}]}{q_{15}} \right) \quad (30)$$

Table 52: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
PGM_v			$5 \cdot 10^8$		<input checked="" type="checkbox"/>
q15			0.058		<input checked="" type="checkbox"/>

6.16 Reaction `light_reaction`

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

Reaction equation



Reactants

Table 53: Properties of each reactant.

Id	Name	SBO
Pi_ch		
ADP_ch		

Product

Table 54: Properties of each product.

Id	Name	SBO
ATP_ch		

Kinetic Law

Derived unit contains undeclared units

$$v_{16} = \frac{\text{Light_on} \cdot \text{LR_vm} \cdot [\text{ADP_ch}] \cdot [\text{Pi_ch}] \cdot \text{vol}(\text{chloroplast})}{([\text{ADP_ch}] + \text{LR_kmADP}) \cdot ([\text{Pi_ch}] + \text{LR_kmPi})} \quad (32)$$

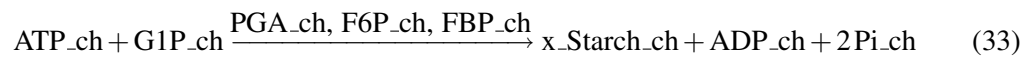
Table 55: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
LR_vm			3500.000		<input checked="" type="checkbox"/>
LR_kmADP			0.014		<input checked="" type="checkbox"/>
LR_kmPi			0.300		<input checked="" type="checkbox"/>

6.17 Reaction E16

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

Reaction equation



Reactants

Table 56: Properties of each reactant.

Id	Name	SBO
ATP_ch		
G1P_ch		

Modifiers

Table 57: Properties of each modifier.

Id	Name	SBO
PGA_ch		
F6P_ch		
FBP_ch		

Products

Table 58: Properties of each product.

Id	Name	SBO
x_Starch_ch		
ADP_ch		
Pi_ch		

Kinetic Law

Derived unit contains undeclared units

$$v_{17} = \frac{\text{StSyn_vm} \cdot [\text{G1P_ch}] \cdot [\text{ATP_ch}] \cdot \text{vol}(\text{chloroplast})}{([\text{G1P_ch}] + \text{stsyn_ch_km1}) \cdot \left(1 + \frac{[\text{ADP_ch}]}{\text{stsyn_ch_Ki}}\right) \cdot ([\text{ATP_ch}] + \text{stsyn_ch_km2}) + \frac{\text{stsyn_ch_km2} \cdot [\text{Pi_ch}]}{\text{stsyn_ch_ka1} \cdot [\text{PGA_ch}]} + \text{stsyn_ch_ka2}}$$

Table 59: Properties of each parameter.

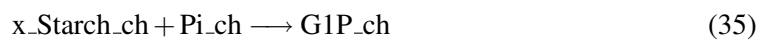
Id	Name	SBO	Value	Unit	Constant
StSyn_vm			40.00		✓
stsyn_ch_km1			0.08		✓
stsyn_ch_Ki			10.00		✓
stsyn_ch_km2			0.08		✓
stsyn_ch_ka1			0.10		✓

Id	Name	SBO	Value	Unit	Constant
stsyn_ch_ka2			0.02		<input checked="" type="checkbox"/>
stsyn_ch_ka3			0.02		<input checked="" type="checkbox"/>

6.18 Reaction E17

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

Reaction equation



Reactants

Table 60: Properties of each reactant.

Id	Name	SBO
x_Starch_ch		
Pi_ch		

Product

Table 61: Properties of each product.

Id	Name	SBO
G1P_ch		

Kinetic Law

Derived unit contains undeclared units

$$v_{18} = \frac{StPase_Vm \cdot [Pi_ch] \cdot vol(chloroplast)}{[Pi_ch] + StPase_km \cdot \left(1 + \frac{[G1P_ch]}{StPase_kiG1P}\right)} \quad (36)$$

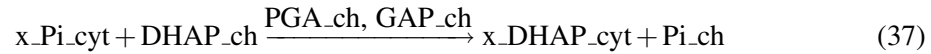
Table 62: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
StPase_Vm			40.00		<input checked="" type="checkbox"/>
StPase_km			0.10		<input checked="" type="checkbox"/>
StPase_kiG1P			0.05		<input checked="" type="checkbox"/>

6.19 Reaction E18_DHAP

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

Reaction equation



Reactants

Table 63: Properties of each reactant.

Id	Name	SBO
x_Pi_cyt		
DHAP_ch		

Modifiers

Table 64: Properties of each modifier.

Id	Name	SBO
PGA_ch		
GAP_ch		

Products

Table 65: Properties of each product.

Id	Name	SBO
x_DHAP_cyt		
Pi_ch		

Kinetic Law

Derived unit contains undeclared units

v_{19}

(38)

$$= \frac{TP_Piap_vm \cdot [DHAP_ch] \cdot vol(chloroplast)}{TP_Piap_kDHAP_ch \cdot \left(1 + \left(1 + \frac{TP_Piap_kPi_cyt}{[x_Pi_cyt]}\right) \cdot \left(\frac{[Pi_ch]}{TP_Piap_kPi_ch} + \frac{[PGA_ch]}{TP_Piap_kPGA_ch} + \frac{[DHAP_ch]}{TP_Piap_kDHAP_ch} + \frac{[GAP_ch]}{TP_Piap_kGAP_ch}\right)\right)}$$

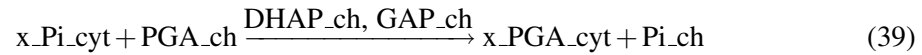
Table 66: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
TP_Piap_vm			250.000		✓
TP_Piap-			0.077		✓
_kDHAP_ch					
TP_Piap_kPi-			0.740		✓
_cyt					
TP_Piap_kPi-			0.630		✓
_ch					
TP_Piap-			0.250		✓
_kPGA_ch					
TP_Piap-			0.075		✓
_kGAP_ch					

6.20 Reaction E18_PGA

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

Reaction equation



Reactants

Table 67: Properties of each reactant.

Id	Name	SBO
x_Pi_cyt		
PGA_ch		

Modifiers

Table 68: Properties of each modifier.

Id	Name	SBO
DHAP_ch		
GAP_ch		

Products

Table 69: Properties of each product.

Id	Name	SBO
x_PGA_cyt		
Pi_ch		

Kinetic Law

Derived unit contains undeclared units

$$v_{20} = \frac{\text{PGA_xpMult} \cdot \text{TP_Piap_vm} \cdot [\text{PGA_ch}] \cdot \text{vol}(\text{chloroplast})}{\text{TP_Piap_kPGA_ch} \cdot \left(1 + \left(1 + \frac{\text{TP_Piap_kPi_cyt}}{[\text{x_Pi_cyt}]}\right) \cdot \left(\frac{[\text{Pi_ch}]}{\text{TP_Piap_kPi_ch}} + \frac{[\text{PGA_ch}]}{\text{TP_Piap_kPGA_ch}} + \frac{[\text{DHAP_ch}]}{\text{TP_Piap_kDHAP_ch}} + \frac{[\text{GAP_ch}]}{\text{TP_Piap_kGAP_ch}}\right)\right)} \quad (40)$$

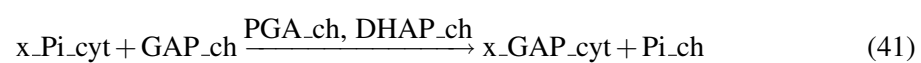
Table 70: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
PGA_xpMult			0.750		✓
TP_Piap_vm			250.000		✓
TP_Piap_kPGA_ch			0.250		✓
TP_Piap_kPi_cyt			0.740		✓
TP_Piap_kPi_ch			0.630		✓
TP_Piap_kDHAP_ch			0.077		✓
TP_Piap_kGAP_ch			0.075		✓

6.21 Reaction E18_GAP

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

Reaction equation



Reactants

Table 71: Properties of each reactant.

Id	Name	SBO
x_Pi_cyt		
GAP_ch		

Modifiers

Table 72: Properties of each modifier.

Id	Name	SBO
PGA_ch		
DHAP_ch		

Products

Table 73: Properties of each product.

Id	Name	SBO
x_GAP_cyt		
Pi_ch		

Kinetic Law

Derived unit contains undeclared units

$$v_{21} = \frac{TP_Piap_vm \cdot [GAP_ch] \cdot vol \text{ (chloroplast)}}{TP_Piap_kGAP_ch \cdot \left(1 + \left(1 + \frac{TP_Piap_kPi_cyt}{[x_Pi_cyt]}\right) \cdot \left(\frac{[Pi_ch]}{TP_Piap_kPi_ch} + \frac{[PGA_ch]}{TP_Piap_kPGA_ch} + \frac{[DHAP_ch]}{TP_Piap_kDHAP_ch} + \frac{[GAP_ch]}{TP_Piap_kGAP_ch}\right)\right)}$$

(42)

Table 74: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
TP_Piap_vm			250.000		✓
TP_Piap-_kGAP_ch			0.075		✓
TP_Piap_kPi-_cyt			0.740		✓

Id	Name	SBO	Value	Unit	Constant
TP_Piap_kPi-_ch			0.630		✓
TP_Piap-_kPGA_ch			0.250		✓
TP_Piap-_kDHAP_ch			0.077		✓

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 `x_CO2`

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

This species takes part in one reaction (as a reactant in [E1](#)), which does not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{d}{dt}x_{\text{CO2}} = 0 \quad (43)$$

7.2 Species `RuBP_ch`

Initial concentration $0.33644 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a reactant in [E1](#) and as a product in [E13](#)).

$$\frac{d}{dt}\text{RuBP}_{\text{ch}} = v_{13} - v_1 \quad (44)$$

7.3 Species `PGA_ch`

Initial concentration $3.35479 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in seven reactions (as a reactant in [E2](#), [E18_PGA](#) and as a product in [E1](#) and as a modifier in [E13](#), [E16](#), [E18_DHAP](#), [E18_GAP](#)).

$$\frac{d}{dt}\text{PGA}_{\text{ch}} = 2v_1 - v_2 - v_{20} \quad (45)$$

7.4 Species ATP_ch

Initial concentration 0.49806 mmol · l⁻¹

This species takes part in four reactions (as a reactant in E2, E13, E16 and as a product in light_reaction).

$$\frac{d}{dt}\text{ATP_ch} = v_{16} - v_2 - v_{13} - v_{17} \quad (46)$$

7.5 Species BPGA_ch

Initial concentration 0.14825 mmol · l⁻¹

This species takes part in two reactions (as a reactant in E3 and as a product in E2).

$$\frac{d}{dt}\text{BPGA_ch} = v_2 - v_3 \quad (47)$$

7.6 Species x_NADPH_ch

Initial concentration 0.21 mmol · l⁻¹

This species takes part in two reactions (as a reactant in E3 and as a modifier in E1), which do not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{d}{dt}x_NADPH_ch = 0 \quad (48)$$

7.7 Species GAP_ch

Initial concentration 0.01334 mmol · l⁻¹

This species takes part in eight reactions (as a reactant in E4, E5, E7, E10, E18_GAP and as a product in E3 and as a modifier in E18_DHAP, E18_PGA).

$$\frac{d}{dt}\text{GAP_ch} = v_3 - v_4 - v_5 - v_7 - v_{10} - v_{21} \quad (49)$$

7.8 Species Pi_ch

Initial concentration 1.5662 mmol · l⁻¹

This species takes part in eleven reactions (as a reactant in light_reaction, E17 and as a product in E3, E6, E9, E16, E18_DHAP, E18_PGA, E18_GAP and as a modifier in E1, E13).

$$\frac{d}{dt}\text{Pi_ch} = v_3 + v_6 + v_9 + 2v_{17} + v_{19} + v_{20} + v_{21} - v_{16} - v_{18} \quad (50)$$

7.9 Species DHAP_ch

Initial concentration 0.29345 mmol · l⁻¹

This species takes part in six reactions (as a reactant in E5, E8, E18_DHAP and as a product in E4 and as a modifier in E18_PGA, E18_GAP).

$$\frac{d}{dt}\text{DHAP_ch} = v_4 - v_5 - v_8 - v_{19} \quad (51)$$

7.10 Species FBP_ch

Initial concentration 0.02776 mmol · l⁻¹

This species takes part in four reactions (as a reactant in E6 and as a product in E5 and as a modifier in E1, E16).

$$\frac{d}{dt}\text{FBP_ch} = v_5 - v_6 \quad (52)$$

7.11 Species F6P_ch

Initial concentration 1.36481 mmol · l⁻¹

This species takes part in four reactions (as a reactant in E7, E14 and as a product in E6 and as a modifier in E16).

$$\frac{d}{dt}\text{F6P_ch} = v_6 - v_7 - v_{14} \quad (53)$$

7.12 Species E4P_ch

Initial concentration 0.41021 mmol · l⁻¹

This species takes part in two reactions (as a reactant in E8 and as a product in E7).

$$\frac{d}{dt}\text{E4P_ch} = v_7 - v_8 \quad (54)$$

7.13 Species X5P_ch

Initial concentration 0.00363 mmol · l⁻¹

This species takes part in three reactions (as a reactant in E12 and as a product in E7, E10).

$$\frac{d}{dt}\text{X5P_ch} = v_7 + v_{10} - v_{12} \quad (55)$$

7.14 Species SBP_ch

Initial concentration 1.56486 mmol · l⁻¹

This species takes part in three reactions (as a reactant in E9 and as a product in E8 and as a modifier in E1).

$$\frac{d}{dt} \text{SBP_ch} = v_8 - v_9 \quad (56)$$

7.15 Species S7P_ch

Initial concentration 0.00541 mmol · l⁻¹

This species takes part in two reactions (as a reactant in E10 and as a product in E9).

$$\frac{d}{dt} \text{S7P_ch} = v_9 - v_{10} \quad (57)$$

7.16 Species R5P_ch

Initial concentration 0.00599 mmol · l⁻¹

This species takes part in two reactions (as a reactant in E11 and as a product in E10).

$$\frac{d}{dt} \text{R5P_ch} = v_{10} - v_{11} \quad (58)$$

7.17 Species Ru5P_ch

Initial concentration 0.00235 mmol · l⁻¹

This species takes part in three reactions (as a reactant in E13 and as a product in E11, E12).

$$\frac{d}{dt} \text{Ru5P_ch} = v_{11} + v_{12} - v_{13} \quad (59)$$

7.18 Species x_Pi_cyt

Initial concentration 0.5 mmol · l⁻¹

This species takes part in three reactions (as a reactant in E18_DHAP, E18_PGA, E18_GAP), which do not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{d}{dt} \text{x_Pi_cyt} = 0 \quad (60)$$

7.19 Species `x_GAP_cyt`

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

This species takes part in one reaction (as a product in [E18_GAP](#)), which does not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{d}{dt}x_{\text{GAP_cyt}} = 0 \quad (61)$$

7.20 Species `G6P_ch`

Initial concentration $3.1396 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a reactant in [E15](#) and as a product in [E14](#)).

$$\frac{d}{dt}G6P_{\text{ch}} = v_{14} - v_{15} \quad (62)$$

7.21 Species `x_NADP_ch`

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

This species takes part in one reaction (as a product in [E3](#)), which does not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{d}{dt}x_{\text{NADP_ch}} = 0 \quad (63)$$

7.22 Species `x_PGA_cyt`

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

This species takes part in one reaction (as a product in [E18_PGA](#)), which does not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{d}{dt}x_{\text{PGA_cyt}} = 0 \quad (64)$$

7.23 Species `ADP_ch`

Initial concentration $0.00149 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in four reactions (as a reactant in [light_reaction](#) and as a product in [E2](#), [E13](#), [E16](#)).

$$\frac{d}{dt}ADP_{\text{ch}} = v_2 + v_{13} + v_{17} - v_{16} \quad (65)$$

7.24 Species $x_{\text{DHAP_cyt}}$

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

This species takes part in one reaction (as a product in [E18_DHAP](#)), which does not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{d}{dt}x_{\text{DHAP_cyt}} = 0 \quad (66)$$

7.25 Species $x_{\text{Proton_ch}}$

Initial concentration $2.512 \cdot 10^{-5} \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in one reaction (as a reactant in [E3](#)), which does not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{d}{dt}x_{\text{Proton_ch}} = 0 \quad (67)$$

7.26 Species $G1P_ch$

Initial concentration $0.18206 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in three reactions (as a reactant in [E16](#) and as a product in [E15](#), [E17](#)).

$$\frac{d}{dt}G1P_ch = v_{15} + v_{18} - v_{17} \quad (68)$$

7.27 Species $x_{\text{Starch_ch}}$

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

This species takes part in two reactions (as a reactant in [E17](#) and as a product in [E16](#)), which do not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{d}{dt}x_{\text{Starch_ch}} = 0 \quad (69)$$

SBML²TeX 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.

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