SBML Model Report

Model name: "Arnold2011_Zhu2009_CalvinCycle"

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1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by the following three authors: Vijayalakshmi Chelliah[1], Anne Arnold[2] and Zoran Nikoloski[3] at October 19th 2011 at 2:52 p. m. and last time modified at April 20th 2012 at 7:51 p. m. Table 1 provides 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	1
species types	0	species	8
events	0	constraints	0
reactions	7	function definitions	2
global parameters	0	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 Trends in Plant Science 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 by Zhu et al. (2009, DOI:10.1016/j.nonrwa.2008.01.021). 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 Compartment

This model contains one compartment.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
`chloroplast`	chloroplast		3	1	litre	☑	

3.1 Compartment `chloroplast`

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

Name chloroplast

4 Species

This model contains eight species. The boundary condition of three of these species is set to `true` so that these species' amount cannot be changed by any reaction. Section 8 provides further details and the derived rates of change of each species.

Table 3: Properties of each species.

Id	Name	Compartment	Derived Unit	Constant	Boundary Condition
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	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☐
Ru5P	Ru5P	chloroplast	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☐
ADP	ADP	chloroplast	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑	☑
ATP	ATP	chloroplast	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑	☑
Pi	Pi	chloroplast	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☑

5 Function definitions

This is an overview of two function definitions.

5.1 Function definition `function_1`

Name Henri-Michaelis-Menten (irreversible)

Arguments substrate, Km, V

Mathematical Expression

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

5.2 Function definition `function_2`

Name MM s2 - reg

Arguments Vm, s1, s2, K1, K2

Mathematical Expression

$$\frac{\mathrm{Vm} \cdot \mathrm{s1} \cdot \mathrm{s2}}{(\mathrm{s1} + \mathrm{K1}) \cdot (\mathrm{s2} + \mathrm{K2})} \tag{2}$$

6 Rule

This is an overview of one rule.

6.1 Rule `Pi`

Rule `Pi` is an assignment rule for species `Pi`:

$$\mathrm{Pi} = 15 - 2 \cdot ([\mathrm{RuBP}] + [\mathrm{DPGA}] + [\mathrm{ATP}]) - ([\mathrm{PGA}] + [\mathrm{GAP}] + [\mathrm{Ru5P}] + [\mathrm{ADP}]) \tag{3}$$

7 Reactions

This model contains seven 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	$\mathrm{RuBP} \longrightarrow 2\,\mathrm{PGA}$	
2	PGA_K	PGA kinase	$\mathrm{PGA} + \mathrm{ATP} \longrightarrow \mathrm{ADP} + \mathrm{DPGA}$	
3	GAP_DH	GAP dehydrogenase	$\mathrm{DPGA} \longrightarrow \mathrm{GAP} + \mathrm{Pi}$	
4	GAP2Ru5P	GAP to Ru5P	$\mathrm{GAP} \longrightarrow 0 \cdot 6\,\mathrm{Ru5P}$	
5	Ru5P_K	Ru5P kinase	$\mathrm{Ru5P} + \mathrm{ATP} \longrightarrow \mathrm{RuBP} + \mathrm{ADP}$	
6	PGA2sink	PGA to sink	$\mathrm{PGA} \longrightarrow \emptyset$	
7	GAP2sink	GAP to sink	$\mathrm{GAP} \longrightarrow \emptyset$	

7.1 Reaction RuBisCO

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

Name RuBisCO

Reaction equation

$$\mathrm{RuBP} \longrightarrow 2\,\mathrm{PGA} \tag{4}$$

Reactant

Table 5: Properties of each reactant.

Id	Name	SBO
RuBP	RuBP	

Product

Table 6: Properties of each product.

Id	Name	SBO
PGA	PGA	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \mathrm{vol}\,(\mathrm{chloroplast}) \cdot \mathrm{function\_1}\,([\mathrm{RuBP}], \mathrm{Km}, \mathrm{V}) \tag{5}$$

$$\mathrm{function\_1}\,(\mathrm{substrate}, \mathrm{Km}, \mathrm{V}) = \frac{\mathrm{V} \cdot \mathrm{substrate}}{\mathrm{Km} + \mathrm{substrate}} \tag{6}$$

$$\mathrm{function\_1}\,(\mathrm{substrate}, \mathrm{Km}, \mathrm{V}) = \frac{\mathrm{V} \cdot \mathrm{substrate}}{\mathrm{Km} + \mathrm{substrate}} \tag{7}$$

Table 7: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Km	Km	0000027	1.00		☑
V	V	0000009	3.78		☑

7.2 Reaction PGA_K

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

Name PGA kinase

Reaction equation

$$\mathrm{PGA} + \mathrm{ATP} \longrightarrow \mathrm{ADP} + \mathrm{DPGA} \tag{8}$$

Reactants

Table 8: Properties of each reactant.

Id	Name	SBO
PGA	PGA	
ATP	ATP	

Products

Table 9: Properties of each product.

Id	Name	SBO
ADP	ADP	
DPGA	DPGA	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \mathrm{vol}\left(\mathrm{chloroplast}\right) \cdot \mathrm{function\_2}\left(\mathrm{Vm}, [\mathrm{PGA}], [\mathrm{ATP}], \mathrm{K1}, \mathrm{K2}\right) \tag{9}$$

$$\mathrm{function\_2}\left(\mathrm{Vm}, \mathrm{s1}, \mathrm{s2}, \mathrm{K1}, \mathrm{K2}\right) = \frac{\mathrm{Vm} \cdot \mathrm{s1} \cdot \mathrm{s2}}{(\mathrm{s1} + \mathrm{K1}) \cdot (\mathrm{s2} + \mathrm{K2})} \tag{10}$$

$$\mathrm{function\_2}\left(\mathrm{Vm}, \mathrm{s1}, \mathrm{s2}, \mathrm{K1}, \mathrm{K2}\right) = \frac{\mathrm{Vm} \cdot \mathrm{s1} \cdot \mathrm{s2}}{(\mathrm{s1} + \mathrm{K1}) \cdot (\mathrm{s2} + \mathrm{K2})} \tag{11}$$

Table 10: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vm	Vm	0000009	11.75		☑
K1	K1	0000009	0.24		☑
K2	K2	0000009	0.39		☑

7.3 Reaction GAP_DH

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

Name GAP dehydrogenase

Reaction equation

$$\mathrm{DPGA} \longrightarrow \mathrm{GAP} + \mathrm{Pi} \tag{12}$$

Reactant

Table 11: Properties of each reactant.

Id	Name	SBO
DPGA	DPGA	

Products

Table 12: Properties of each product.

Id	Name	SBO
GAP	GAP	
Pi	Pi	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \mathrm{vol}\left(\mathrm{chloroplast}\right) \cdot \mathrm{function\_1}\left(\left[\mathrm{DPGA}\right], \mathrm{Km}, \mathrm{V}\right) \tag{13}$$

$$\mathrm{function\_1}\left(\mathrm{substrate}, \mathrm{Km}, \mathrm{V}\right) = \frac{\mathrm{V} \cdot \mathrm{substrate}}{\mathrm{Km} + \mathrm{substrate}} \tag{14}$$

$$\mathrm{function\_1}\left(\mathrm{substrate}, \mathrm{Km}, \mathrm{V}\right) = \frac{\mathrm{V} \cdot \mathrm{substrate}}{\mathrm{Km} + \mathrm{substrate}} \tag{15}$$

Table 13: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Km	Km	0000027	0.50		☑
V	V	0000009	5.04		☑

7.4 Reaction GAP2Ru5P

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

Name GAP to Ru5P

Reaction equation

$$\mathrm{GAP} \longrightarrow 0{\cdot}6\,\mathrm{Ru5P} \tag{16}$$

Reactant

Table 14: Properties of each reactant.

Id	Name	SBO
GAP	GAP	

Product

Table 15: Properties of each product.

Id	Name	SBO
Ru5P	Ru5P	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \mathrm{vol}\left(\mathrm{chloroplast}\right) \cdot \mathrm{function\_1}\left([\mathrm{GAP}], \mathrm{Km}, \mathrm{V}\right) \tag{17}$$

$$\mathrm{function\_1}\left(\mathrm{substrate}, \mathrm{Km}, \mathrm{V}\right) = \frac{\mathrm{V} \cdot \mathrm{substrate}}{\mathrm{Km} + \mathrm{substrate}} \tag{18}$$

$$\mathrm{function\_1}\left(\mathrm{substrate}, \mathrm{Km}, \mathrm{V}\right) = \frac{\mathrm{V} \cdot \mathrm{substrate}}{\mathrm{Km} + \mathrm{substrate}} \tag{19}$$

Table 16: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Km	Km	0000027	0.84		☑
V	V	0000009	3.05		☑

7.5 Reaction Ru5P_K

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

Name Ru5P kinase

Reaction equation

$$\mathrm{Ru5P} + \mathrm{ATP} \longrightarrow \mathrm{RuBP} + \mathrm{ADP} \tag{20}$$

Reactants

Table 17: Properties of each reactant.

Id	Name	SBO
Ru5P	Ru5P	
ATP	ATP	

Products

Table 18: Properties of each product.

Id	Name	SBO
RuBP	RuBP	
ADP	ADP	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \mathrm{vol}\left(\mathrm{chloroplast}\right) \cdot \mathrm{function\_2}\left(\mathrm{Vm}, [\mathrm{Ru5P}], [\mathrm{ATP}], \mathrm{K1}, \mathrm{K2}\right) \tag{21}$$

$$\mathrm{function\_2}\left(\mathrm{Vm}, \mathrm{s1}, \mathrm{s2}, \mathrm{K1}, \mathrm{K2}\right) = \frac{\mathrm{Vm} \cdot \mathrm{s1} \cdot \mathrm{s2}}{(\mathrm{s1} + \mathrm{K1}) \cdot (\mathrm{s2} + \mathrm{K2})} \tag{22}$$

$$\mathrm{function\_2}\left(\mathrm{Vm}, \mathrm{s1}, \mathrm{s2}, \mathrm{K1}, \mathrm{K2}\right) = \frac{\mathrm{Vm} \cdot \mathrm{s1} \cdot \mathrm{s2}}{(\mathrm{s1} + \mathrm{K1}) \cdot (\mathrm{s2} + \mathrm{K2})} \tag{23}$$

Table 19: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vm	Vm	0000009	8.000		☑
K1	K1	0000009	0.150		☑
K2	K2	0000009	0.059		☑

7.6 Reaction PGA2sink

This is an irreversible reaction of one reactant forming no product.

Name PGA to sink

Notes changed velocity in accordance with the authors (Lei et al. (2011))

Reaction equation

$$\mathrm{PGA} \longrightarrow \emptyset \tag{24}$$

Reactant

Table 20: Properties of each reactant.

Id	Name	SBO
PGA	PGA	

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \mathrm{vol}\left(\mathrm{chloroplast}\right) \cdot \mathrm{function\_1}\left(\left[\mathrm{PGA}\right], \mathrm{Km}, \mathrm{V}\right) \tag{25}$$

$$\mathrm{function\_1}\left(\mathrm{substrate}, \mathrm{Km}, \mathrm{V}\right) = \frac{\mathrm{V} \cdot \mathrm{substrate}}{\mathrm{Km} + \mathrm{substrate}} \tag{26}$$

$$\mathrm{function\_1}\left(\mathrm{substrate}, \mathrm{Km}, \mathrm{V}\right) = \frac{\mathrm{V} \cdot \mathrm{substrate}}{\mathrm{Km} + \mathrm{substrate}} \tag{27}$$

Table 21: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Km	Km	0000027	0.75		☑
V	V	0000009	3.00		☑

7.7 Reaction GAP2sink

This is an irreversible reaction of one reactant forming no product.

Name GAP to sink

Reaction equation

$$\mathrm{GAP} \longrightarrow \emptyset \tag{28}$$

Reactant

Table 22: Properties of each reactant.

Id	Name	SBO
GAP	GAP	

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \mathrm{vol}\left(\mathrm{chloroplast}\right) \cdot \mathrm{function\_1}\left(\left[\mathrm{GAP}\right], \mathrm{Km}, \mathrm{V}\right) \tag{29}$$

$$\mathrm{function\_1}\left(\mathrm{substrate}, \mathrm{Km}, \mathrm{V}\right) = \frac{\mathrm{V} \cdot \mathrm{substrate}}{\mathrm{Km} + \mathrm{substrate}} \tag{30}$$

$$\mathrm{function\_1}\left(\mathrm{substrate}, \mathrm{Km}, \mathrm{V}\right) = \frac{\mathrm{V} \cdot \mathrm{substrate}}{\mathrm{Km} + \mathrm{substrate}} \tag{31}$$

Table 23: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Km	Km	0000027	5.0		☑
V	V	0000009	0.1		☑

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 two reactions (as a reactant in RuBisCO and as a product in Ru5P_K).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{RuBP} = v_5 - v_1 \tag{32}$$

8.2 Species PGA

Name PGA

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

This species takes part in three reactions (as a reactant in PGA_K, PGA2sink and as a product in RuBisCO).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{PGA} = 2\,v_1 - v_2 - v_6 \tag{33}$$

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).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{DPGA} = v_2 - v_3 \tag{34}$$

8.4 Species GAP

Name GAP

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

This species takes part in three reactions (as a reactant in GAP2Ru5P, GAP2sink and as a product in GAP_DH).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{GAP} = v_3 - v_4 - v_7 \tag{35}$$

8.5 Species Ru5P

Name Ru5P

Initial concentration $0.0501\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in Ru5P_K and as a product in GAP2Ru5P).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Ru5P} = 0.6\, v_4 - v_5 \tag{36}$$

8.6 Species ADP

Name ADP

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

This species takes part in two reactions (as a product in PGA_K, Ru5P_K), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ADP} = 0 \tag{37}$$

8.7 Species ATP

Name ATP

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

This species takes part in two reactions (as a reactant in PGA_K, Ru5P_K), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ATP} = 0 \tag{38}$$

8.8 Species Pi

Name Pi

Initial concentration $6.3477\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

Involved in rule Pi

This species takes part in one reaction (as a product in GAP_DH). Not this but one rule determines the species' quantity because this species is on the boundary of the reaction system.

A Glossary of Systems Biology Ontology Terms

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

SBO:0000027 Michaelis constant: Substrate concentration at which the velocity of reaction is half its maximum. Michaelis constant is an experimental parameter. According to the underlying molecular mechanism it can be interpreted differently in terms of microscopic constants

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.

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