SBML Model Report

Model name: "Arnold2011_Medlyn2002-_RuBisCO-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 2:50 p. m. and last time modified at April 20th 2012 at 7:53 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	1
species types	0	species	6
events	0	constraints	0
reactions	4	function definitions	4
global parameters	14	unit definitions	1
rules	6	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 with focus on the RuBisCO reaction by Medlyn et al. (2002, DOI:10.1046/j.1365-3040.2002.00891.x). The parameter values are widely taken from Farquhar et al. (1980, DOI:10.1007/BF00386231). 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 four are predefined by SBML and not mentioned in the model.

2.1 Unit `substance`

Definition mmol

2.2 Unit `volume`

Notes Litre is the predefined SBML unit for `volume`.

Definition l

2.3 Unit `area`

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

Definition m^2

2.4 Unit `length`

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

Definition m

2.5 Unit `time`

Notes Second is the predefined SBML unit for `time`.

Definition s

3 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 six species. The boundary condition of four 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 Condition
`RuBP`	RuBP	`chloroplast`	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑	☑
`PGA`	PGA	`chloroplast`	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☐
`NADPH`	NADPH	`chloroplast`	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☐
`CO2`	CO2	`chloroplast`	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑	☑
`O2`	O2	`chloroplast`	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑	☑
`NADP`	NADP	`chloroplast`	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☑

5 Parameters

This model contains 14 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Rp	Rp		3.200		☑
Nt	Nt	0000009	0.500		☑
alpha	alpha	0000009	0.300		☑
Q	Q	0000009	1000.000		☑
J	J	0000009	4.858		☐
Gamma	Gamma	0000009	42.893		☑
teta	teta	0000009	0.900		☑
Vcmax	Vcmax	0000009	2.532		☑
Vomax	Vomax		0.532		☐
Kc	Kc	0000009	406.066		☑
Ko	Ko		276.900		☑
Vj	Vj	0000009	0.900		☐
phi	phi	0000009	0.264		☐
Vc	Vc	0000009	0.647		☐

6 Function definitions

This is an overview of four function definitions.

6.1 Function definition PGA_consumption

Name PGA consumption

Arguments S1, Rp, R, Nt, Vc

Mathematical Expression

$$\frac{S1}{Rp} \cdot \frac{R}{Nt} \cdot Vc \tag{1}$$

6.2 Function definition NADPH_production

Name NADPH production

Arguments j, S1, Nt

Mathematical Expression

$$\frac{j}{2} \cdot \frac{S1}{Nt} \tag{2}$$

6.3 Function definition carboxylation

Name Carboxylation

Arguments Vc, Vj

Mathematical Expression

$$\frac{\mathrm{Vc} + \mathrm{Vj} - |\mathrm{Vc} - \mathrm{Vj}|}{2} \tag{3}$$

6.4 Function definition oxygenation

Name Oxygenation

Arguments phi, Vc, Vj

Mathematical Expression

$$\frac{\mathrm{phi} \cdot (\mathrm{Vc} + \mathrm{Vj} - |\mathrm{Vc} - \mathrm{Vj}|)}{2} \tag{4}$$

7 Rules

This is an overview of six rules.

7.1 Rule J

Rule J is an assignment rule for parameter J:

$$\mathrm{J} = \frac{\frac{\mathrm{alpha} \cdot \mathrm{Q}}{10 - 9 \cdot \mathrm{teta}}}{65 \cdot 0.5} \tag{5}$$

7.2 Rule Vj

Rule Vj is an assignment rule for parameter Vj:

$$\mathrm{Vj} = \frac{\frac{\mathrm{J}}{4} \cdot [\mathrm{CO2}]}{[\mathrm{CO2}] + 2 \cdot \mathrm{Gamma}} \tag{6}$$

7.3 Rule Vc

Rule Vc is an assignment rule for parameter Vc:

$$\mathrm{Vc} = \frac{\mathrm{Vcmax} \cdot [\mathrm{CO2}]}{\left(1 + \frac{[\mathrm{O2}]}{\mathrm{Ko}}\right) \cdot \mathrm{Kc} + [\mathrm{CO2}]} \tag{7}$$

7.4 Rule NADP

Rule NADP is an assignment rule for species NADP:

$$\mathrm{NADP} = \mathrm{Nt} - [\mathrm{NADPH}] \tag{8}$$

7.5 Rule Vomax

Rule Vomax is an assignment rule for parameter Vomax:

$$\mathrm{Vomax} = 0.21 \cdot \mathrm{Vcmax} \tag{9}$$

7.6 Rule phi

Rule phi is an assignment rule for parameter phi:

$$\mathrm{phi} = \frac{0.21 \cdot \frac{[\mathrm{O2}]}{\mathrm{Ko}}}{\frac{[\mathrm{CO2}]}{\mathrm{Kc}}} \tag{10}$$

8 Reactions

This model contains four 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

№	Id	Name	Reaction Equation	SBO
1	PGA_prod_Vc	PGA production - v_c	$\mathrm{RuBP} + \mathrm{CO2} + 2\,\mathrm{NADPH} \longrightarrow 2\,\mathrm{PGA}$	
2	PGA_prod_Vo	PGA production - v_o	$\mathrm{RuBP} + \mathrm{O2} + 2\,\mathrm{NADPH} \longrightarrow 1 \cdot 5\,\mathrm{PGA}$	
3	PGA_cons	PGA consumption	$\mathrm{PGA} \xrightarrow{\mathrm{NADPH}} \mathrm{RuBP}$	
4	NADPH_prod	NADPH production	$\mathrm{NADP} \longrightarrow \mathrm{NADPH}$	

8.1 Reaction PGA_prod_Vc

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

Name PGA production - v_c

Reaction equation

$$\mathrm{RuBP} + \mathrm{CO2} + 2\,\mathrm{NADPH} \longrightarrow 2\,\mathrm{PGA} \tag{11}$$

Reactants

Table 6: Properties of each reactant.

Id	Name	SBO
RuBP	RuBP	
CO2	CO2	
NADPH	NADPH	

Product

Table 7: Properties of each product.

Id	Name	SBO
PGA	PGA	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \mathrm{vol}\,(\mathrm{chloroplast}) \cdot \mathrm{carboxylation}\,(\mathrm{Vc}, \mathrm{Vj}) \tag{12}$$

$$\mathrm{carboxylation}\,(\mathrm{Vc}, \mathrm{Vj}) = \frac{\mathrm{Vc} + \mathrm{Vj} - |\mathrm{Vc} - \mathrm{Vj}|}{2} \tag{13}$$

$$\mathrm{carboxylation}\,(\mathrm{Vc}, \mathrm{Vj}) = \frac{\mathrm{Vc} + \mathrm{Vj} - |\mathrm{Vc} - \mathrm{Vj}|}{2} \tag{14}$$

8.2 Reaction PGA_prod_Vo

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

Name PGA production - v_o

Reaction equation

$$\mathrm{RuBP} + \mathrm{O2} + 2\,\mathrm{NADPH} \longrightarrow 1{\cdot}5\,\mathrm{PGA} \tag{15}$$

Reactants

Table 8: Properties of each reactant.

Id	Name	SBO
RuBP	RuBP	
O2	O2	
NADPH	NADPH	

Product

Table 9: Properties of each product.

Id	Name	SBO
PGA	PGA	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \mathrm{vol}\,(\mathrm{chloroplast}) \cdot \mathrm{oxygenation}\,(\mathrm{phi}, \mathrm{Vc}, \mathrm{Vj}) \tag{16}$$

$$\mathrm{oxygenation}\,(\mathrm{phi}, \mathrm{Vc}, \mathrm{Vj}) = \frac{\mathrm{phi} \cdot (\mathrm{Vc} + \mathrm{Vj} - |\mathrm{Vc} - \mathrm{Vj}|)}{2} \tag{17}$$

$$\mathrm{oxygenation}\,(\mathrm{phi}, \mathrm{Vc}, \mathrm{Vj}) = \frac{\mathrm{phi} \cdot (\mathrm{Vc} + \mathrm{Vj} - |\mathrm{Vc} - \mathrm{Vj}|)}{2} \tag{18}$$

8.3 Reaction PGA_cons

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

Name PGA consumption

Reaction equation

$$\mathrm{PGA} \xrightarrow{\mathrm{NADPH}} \mathrm{RuBP} \tag{19}$$

Reactant

Table 10: Properties of each reactant.

Id	Name	SBO
PGA	PGA	

Modifier

Table 11: Properties of each modifier.

Id	Name	SBO
NADPH	NADPH	

Product

Table 12: Properties of each product.

Id	Name	SBO
RuBP	RuBP	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \text{vol}\left(\text{chloroplast}\right) \cdot \text{PGA\_consumption}\left(\left[\text{PGA}\right], \text{Rp}, \left[\text{NADPH}\right], \text{Nt}, \text{Vcmax}\right) \tag{20}$$

$$\text{PGA\_consumption}\left(\text{S1}, \text{Rp}, \text{R}, \text{Nt}, \text{Vc}\right) = \frac{\text{S1}}{\text{Rp}} \cdot \frac{\text{R}}{\text{Nt}} \cdot \text{Vc} \tag{21}$$

$$\text{PGA\_consumption}\left(\text{S1}, \text{Rp}, \text{R}, \text{Nt}, \text{Vc}\right) = \frac{\text{S1}}{\text{Rp}} \cdot \frac{\text{R}}{\text{Nt}} \cdot \text{Vc} \tag{22}$$

8.4 Reaction NADPH_prod

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

Name NADPH production

Reaction equation

$$\text{NADP} \longrightarrow \text{NADPH} \tag{23}$$

Reactant

Table 13: Properties of each reactant.

Id	Name	SBO
NADP	NADP	

Product

Table 14: Properties of each product.

Id	Name	SBO
NADPH	NADPH	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \mathrm{vol}\,(\mathrm{chloroplast}) \cdot \mathrm{NADPH\_production}\,(\mathrm{J}, [\mathrm{NADP}], \mathrm{Nt}) \tag{24}$$

$$\mathrm{NADPH\_production}\,(\mathrm{j}, \mathrm{S1}, \mathrm{Nt}) = \frac{\mathrm{j}}{2} \cdot \frac{\mathrm{S1}}{\mathrm{Nt}} \tag{25}$$

$$\mathrm{NADPH\_production}\,(\mathrm{j}, \mathrm{S1}, \mathrm{Nt}) = \frac{\mathrm{j}}{2} \cdot \frac{\mathrm{S1}}{\mathrm{Nt}} \tag{26}$$

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

This species takes part in three reactions (as a reactant in PGA_prod_Vc, PGA_prod_Vo and as a product in PGA_cons), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{RuBP} = 0 \tag{27}$$

9.2 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_cons and as a product in PGA_prod_Vc, PGA_prod_Vo).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{PGA} = 2\,v_1 + 1.5\,v_2 - v_3 \tag{28}$$

9.3 Species NADPH

Name NADPH

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

This species takes part in four reactions (as a reactant in PGA_prod_Vc, PGA_prod_Vo and as a product in NADPH_prod and as a modifier in PGA_cons).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{NADPH} = v_4 - 2\,v_1 - 2\,v_2 \tag{29}$$

9.4 Species CO2

Name CO2

Notes 0.7* 350 [bar] (p. 1172)

Initial concentration $245\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{CO2} = 0 \tag{30}$$

9.5 Species O2

Name O2

Notes [mbar]

Initial concentration $210\ \mathrm{mmol} \cdot \mathrm{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{O2} = 0 \tag{31}$$

9.6 Species NADP

Name NADP

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

Involved in rule NADP

This species takes part in one reaction (as a reactant in NADPH_prod). 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

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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