

SBML Model Report

Model name: “Arnold2011_Schultz2003- _RuBisCO-CalvinCycle”



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 Chelliah¹, Anne Arnold² and Zoran Nikoloski³ at October 19th 2011 at 2:51 p. m. and last time modified at April 20th 2012 at 7:52 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	20	unit definitions	1
rules	7	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 Schultz (2003, [DOI:10.1071/FP02146](#)). The parameter values are partly taken from Farquhar et al. (1980, [DOI:10.1007/BF00386231](#)) and Medlyn et al. (2002, [DOI:10.1046/j.1365-3040.2002.00891.x](#)). 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 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 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	<input checked="" type="checkbox"/>	

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 Condi- tion
RuBP	RuBP	chloroplast	$\text{mmol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
PGA	PGA	chloroplast	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
NADPH	NADPH	chloroplast	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
CO2	CO2	chloroplast	$\text{mmol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
O2	O2	chloroplast	$\text{mmol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>
NADP	NADP	chloroplast	$\text{mmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input checked="" type="checkbox"/>

5 Parameters

This model contains 20 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Rp	Rp	0000009	3.200		<input checked="" type="checkbox"/>
Nt	Nt	0000009	0.500		<input checked="" type="checkbox"/>
alpha	alpha	0000009	0.190		<input checked="" type="checkbox"/>
J	J	0000009	2.988		<input type="checkbox"/>
Jmax	Jmax	0000009	112.990		<input checked="" type="checkbox"/>
Gamma	Gamma	0000009	3.817		<input checked="" type="checkbox"/>
PPFD	PPFD	0000196	1000.000		<input checked="" type="checkbox"/>
Vcmax	Vcmax	0000009	1.475		<input checked="" type="checkbox"/>
Kc	Kc	0000009	27.854		<input checked="" type="checkbox"/>
Ko	Ko	0000009	41.947		<input checked="" type="checkbox"/>
phi	phi	0000009	0.117		<input type="checkbox"/>
TPU	TPU	0000196	0.228		<input checked="" type="checkbox"/>
g0	g0	0000009	0.469		<input checked="" type="checkbox"/>
h	h	0000009	0.600		<input checked="" type="checkbox"/>
k	k	0000009	118.690		<input checked="" type="checkbox"/>
Rd	Rd	0000009	0.006		<input checked="" type="checkbox"/>
v_c	v_c	0000009	0.612		<input type="checkbox"/>
Vc	Vc	0000009	0.666		<input type="checkbox"/>
Vj	Vj	0000009	0.612		<input type="checkbox"/>
Vp	Vp	0000009	0.768		<input type="checkbox"/>

6 Function definitions

This is an overview of four function definitions.

6.1 Function definition `NADPH_production`

Name NADPH production

Arguments j, S1, Nt

Mathematical Expression

$$\frac{j}{2} \cdot \frac{S1}{Nt} \quad (1)$$

6.2 Function definition carboxylation

Name Carboxylation

Arguments V_c , V_j , V_p

Mathematical Expression

$$\frac{\frac{V_c + V_j - |V_c - V_j|}{2} + V_p - \left| \frac{V_c + V_j - |V_c - V_j|}{2} - V_p \right|}{2} \quad (2)$$

6.3 Function definition PGA_consumption

Name PGA consumption

Arguments S_1 , R_p , R , N_t , V_c

Mathematical Expression

$$\frac{S_1}{R_p} \cdot \frac{R}{N_t} \cdot V_c \quad (3)$$

6.4 Function definition oxygenation

Name Oxygenation

Arguments ϕ , V_c , V_j , V_p

Mathematical Expression

$$\frac{\phi \cdot \left(\frac{V_c + V_j - |V_c - V_j|}{2} + V_p - \left| \frac{V_c + V_j - |V_c - V_j|}{2} - V_p \right| \right)}{2} \quad (4)$$

7 Rules

This is an overview of seven rules.

7.1 Rule J

Rule J is an assignment rule for parameter J:

$$J = \frac{\frac{\alpha \cdot \text{PPFD}}{\sqrt{2}}}{65 \cdot 0.5} \quad (5)$$

7.2 Rule NADP

Rule NADP is an assignment rule for species NADP:

$$\text{NADP} = N_t - [\text{NADPH}] \quad (6)$$

7.3 Rule V_j

Rule V_j is an assignment rule for parameter V_j :

$$V_j = \frac{J}{4} \quad (7)$$

$$\begin{aligned} & \frac{[CO_2] - 1.6 \cdot \frac{\frac{1}{2} \cdot \left(\frac{1.6 \cdot \left(\frac{J}{4} - Rd \right) + \left(\frac{k \cdot h}{[CO_2]} \cdot Rd + g_0 \right) \cdot ([CO_2] + 2 \cdot \text{Gamma}) + \frac{[CO_2]}{4} \cdot (\text{Gamma} - [CO_2])}{1.6 - \frac{k \cdot h}{[CO_2]} \cdot ([CO_2] + 2 \cdot \text{Gamma})} + \sqrt{2} \right)}{g_0 + \frac{k \cdot h}{[CO_2]} \cdot \frac{1}{2} \cdot \left(\frac{1.6 \cdot \left(\frac{J}{4} - Rd \right) + \left(\frac{k \cdot h}{[CO_2]} \cdot Rd + g_0 \right) \cdot ([CO_2] + 2 \cdot \text{Gamma}) + \frac{[CO_2]}{4} \cdot (\text{Gamma} - [CO_2])}{1.6 - \frac{k \cdot h}{[CO_2]} \cdot ([CO_2] + 2 \cdot \text{Gamma})} + \sqrt{2} \right)}}{[CO_2] - 1.6 \cdot \frac{\frac{1}{2} \cdot \left(\frac{1.6 \cdot \left(\frac{J}{4} - Rd \right) + \left(\frac{k \cdot h}{[CO_2]} \cdot Rd + g_0 \right) \cdot ([CO_2] + 2 \cdot \text{Gamma}) + \frac{[CO_2]}{4} \cdot (\text{Gamma} - [CO_2])}{1.6 - \frac{k \cdot h}{[CO_2]} \cdot ([CO_2] + 2 \cdot \text{Gamma})} + \sqrt{2} \right)}{g_0 + \frac{k \cdot h}{[CO_2]} \cdot \frac{1}{2} \cdot \left(\frac{1.6 \cdot \left(\frac{J}{4} - Rd \right) + \left(\frac{k \cdot h}{[CO_2]} \cdot Rd + g_0 \right) \cdot ([CO_2] + 2 \cdot \text{Gamma}) + \frac{[CO_2]}{4} \cdot (\text{Gamma} - [CO_2])}{1.6 - \frac{k \cdot h}{[CO_2]} \cdot ([CO_2] + 2 \cdot \text{Gamma})} + \sqrt{2} \right)}} + 2 \cdot \text{Gamma} \end{aligned}$$

7.4 Rule V_c

Rule V_c is an assignment rule for parameter V_c :

$$V_c = V_{cmax} \quad (8)$$

$$\begin{aligned} & \frac{[CO_2] - 1.6 \cdot \frac{\frac{1}{2} \cdot \left(\frac{1.6 \cdot (V_{cmax} - Rd) + \left(\frac{k \cdot h}{[CO_2]} \cdot Rd + g_0 \right) \cdot \left([CO_2] + K_c \cdot \left(1 + \frac{[O_2]}{K_o} \right) \right) + \frac{k \cdot h}{[CO_2]} \cdot V_{cmax} \cdot (\text{Gamma} - [CO_2])}{1.6 - \frac{k \cdot h}{[CO_2]} \cdot \left([CO_2] + K_c \cdot \left(1 + \frac{[O_2]}{K_o} \right) \right)} + \sqrt{2} \right)}{g_0 + \frac{k \cdot h}{[CO_2]} \cdot \frac{1}{2} \cdot \left(\frac{1.6 \cdot (V_{cmax} - Rd) + \left(\frac{k \cdot h}{[CO_2]} \cdot Rd + g_0 \right) \cdot \left([CO_2] + K_c \cdot \left(1 + \frac{[O_2]}{K_o} \right) \right) + \frac{k \cdot h}{[CO_2]} \cdot V_{cmax} \cdot (\text{Gamma} - [CO_2])}{1.6 - \frac{k \cdot h}{[CO_2]} \cdot \left([CO_2] + K_c \cdot \left(1 + \frac{[O_2]}{K_o} \right) \right)} + \sqrt{2} \right)}}{[CO_2] - 1.6 \cdot \frac{\frac{1}{2} \cdot \left(\frac{1.6 \cdot (V_{cmax} - Rd) + \left(\frac{k \cdot h}{[CO_2]} \cdot Rd + g_0 \right) \cdot \left([CO_2] + K_c \cdot \left(1 + \frac{[O_2]}{K_o} \right) \right) + \frac{k \cdot h}{[CO_2]} \cdot V_{cmax} \cdot (\text{Gamma} - [CO_2])}{1.6 - \frac{k \cdot h}{[CO_2]} \cdot \left([CO_2] + K_c \cdot \left(1 + \frac{[O_2]}{K_o} \right) \right)} + \sqrt{2} \right)}{g_0 + \frac{k \cdot h}{[CO_2]} \cdot \frac{1}{2} \cdot \left(\frac{1.6 \cdot (V_{cmax} - Rd) + \left(\frac{k \cdot h}{[CO_2]} \cdot Rd + g_0 \right) \cdot \left([CO_2] + K_c \cdot \left(1 + \frac{[O_2]}{K_o} \right) \right) + \frac{k \cdot h}{[CO_2]} \cdot V_{cmax} \cdot (\text{Gamma} - [CO_2])}{1.6 - \frac{k \cdot h}{[CO_2]} \cdot \left([CO_2] + K_c \cdot \left(1 + \frac{[O_2]}{K_o} \right) \right)} + \sqrt{2} \right)}} + K_c \cdot \left(1 + \frac{[O_2]}{K_o} \right) \end{aligned}$$

7.5 Rule V_p

Rule V_p is an assignment rule for parameter V_p :

$$V_p = 3 \cdot TPU \cdot \frac{[CO_2] - 1.6 \cdot \frac{\frac{1}{2} \cdot \left(\frac{1.6 \cdot (3 \cdot TPU - Rd) + \left(\frac{k \cdot h}{[CO_2]} \cdot Rd + g_0 \right) \cdot ([CO_2] - Gamma) - k \cdot h \cdot 3 \cdot TPU}{1.6 - \frac{k \cdot h}{[CO_2]} \cdot ([CO_2] - Gamma)} + \sqrt{2} \right)}{g_0 + \frac{k \cdot h}{[CO_2]} \cdot \frac{1}{2} \cdot \left(\frac{1.6 \cdot (3 \cdot TPU - Rd) + \left(\frac{k \cdot h}{[CO_2]} \cdot Rd + g_0 \right) \cdot ([CO_2] - Gamma) - k \cdot h \cdot 3 \cdot TPU}{1.6 - \frac{k \cdot h}{[CO_2]} \cdot ([CO_2] - Gamma)} + \sqrt{2} \right)}}{\frac{1}{2} \cdot \left(\frac{1.6 \cdot (3 \cdot TPU - Rd) + \left(\frac{k \cdot h}{[CO_2]} \cdot Rd + g_0 \right) \cdot ([CO_2] - Gamma) - k \cdot h \cdot 3 \cdot TPU}{1.6 - \frac{k \cdot h}{[CO_2]} \cdot ([CO_2] - Gamma)} + \sqrt{2} \right)} - Gamma} \quad (9)$$

7.6 Rule v_c

Rule v_c is an assignment rule for parameter v_c :

$$v_c = \frac{\left| \frac{|V_c + V_j| - |V_c - V_j|}{2} + V_p \right| - \left| \frac{|V_c + V_j| - |V_c - V_j|}{2} - V_p \right|}{2} \quad (10)$$

7.7 Rule ϕ

Rule ϕ is an assignment rule for parameter ϕ :

$$\phi = \frac{0.21 \cdot \frac{\left(g_0 + \frac{h \cdot k}{[CO_2]} \cdot (v_c - Rd) \right) \cdot [O_2]}{K_o}}{\frac{g_0 + (h \cdot k - 1.6) \cdot (v_c - Rd)}{K_c}} \quad (11)$$

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

Nº	Id	Name	Reaction Equation	SBO
1	PGA_prod_Vc	PGA production - v_c	$\text{RuBP} + \text{CO}_2 + 2 \text{NADPH} \xrightarrow{\text{O}_2} 2 \text{PGA}$	
2	PGA_prod_Vo	PGA production - v_o	$\text{RuBP} + \text{O}_2 + 2 \text{NADPH} \xrightarrow{\text{CO}_2} 1 \cdot 5 \text{PGA}$	
3	PGA_cons	PGA consumption	$\text{PGA} \xrightarrow{\text{NADPH}} \text{RuBP}$	
4	NADPH_prod	NADPH production	$\text{NADP} \longrightarrow \text{NADPH}$	

8.1 Reaction `PGA_prod_Vc`

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

Name PGA production - `v_c`

Reaction equation



Reactants

Table 6: Properties of each reactant.

Id	Name	SBO
RuBP	RuBP	
CO2	CO2	
NADPH	NADPH	

Modifier

Table 7: Properties of each modifier.

Id	Name	SBO
O2	O2	

Product

Table 8: Properties of each product.

Id	Name	SBO
PGA	PGA	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \text{vol}(\text{chloroplast}) \cdot \text{carboxylation}(\text{Vc}, \text{Vj}, \text{Vp}) \quad (13)$$

$$\text{carboxylation}(\text{Vc}, \text{Vj}, \text{Vp}) = \frac{\frac{\text{Vc} + \text{Vj} - |\text{Vc} - \text{Vj}|}{2} + \text{Vp} - \left| \frac{\text{Vc} + \text{Vj} - |\text{Vc} - \text{Vj}|}{2} - \text{Vp} \right|}{2} \quad (14)$$

$$\text{carboxylation}(V_c, V_j, V_p) = \frac{\frac{V_c + V_j - |V_c - V_j|}{2} + V_p - \left| \frac{V_c + V_j - |V_c - V_j|}{2} - V_p \right|}{2} \quad (15)$$

8.2 Reaction PGA_prod_Vo

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

Name PGA production - v_o

Reaction equation



Reactants

Table 9: Properties of each reactant.

Id	Name	SBO
RuBP	RuBP	
O2	O2	
NADPH	NADPH	

Modifier

Table 10: Properties of each modifier.

Id	Name	SBO
C02	CO2	

Product

Table 11: Properties of each product.

Id	Name	SBO
PGA	PGA	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \text{vol}(\text{chloroplast}) \cdot \text{oxygenation}(\text{phi}, V_c, V_j, V_p) \quad (17)$$

$$\text{oxygenation}(\text{phi}, V_c, V_j, V_p) = \frac{\text{phi} \cdot \left(\frac{V_c + V_j - |V_c - V_j|}{2} + V_p - \left| \frac{V_c + V_j - |V_c - V_j|}{2} - V_p \right| \right)}{2} \quad (18)$$

$$\text{oxygenation}(\text{phi}, V_c, V_j, V_p) = \frac{\text{phi} \cdot \left(\frac{V_c + V_j - |V_c - V_j|}{2} + V_p - \left| \frac{V_c + V_j - |V_c - V_j|}{2} - V_p \right| \right)}{2} \quad (19)$$

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



Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
PGA	PGA	

Modifier

Table 13: Properties of each modifier.

Id	Name	SBO
NADPH	NADPH	

Product

Table 14: Properties of each product.

Id	Name	SBO
RuBP	RuBP	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \text{vol}(\text{chloroplast}) \cdot \text{PGA_consumption}([\text{PGA}], R_p, [\text{NADPH}], N_t, V_{\text{cmax}}) \quad (21)$$

$$\text{PGA_consumption}(S_1, R_p, R, N_t, V_c) = \frac{S_1}{R_p} \cdot \frac{R}{N_t} \cdot V_c \quad (22)$$

$$\text{PGA_consumption}(S_1, R_p, R, N_t, V_c) = \frac{S_1}{R_p} \cdot \frac{R}{N_t} \cdot V_c \quad (23)$$

8.4 Reaction NADPH_prod

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

Name NADPH production

Reaction equation



Reactant

Table 15: Properties of each reactant.

Id	Name	SBO
NADP	NADP	

Product

Table 16: Properties of each product.

Id	Name	SBO
NADPH	NADPH	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \text{vol}(\text{chloroplast}) \cdot \text{NADPH_production}(J, [\text{NADP}], N_t) \quad (25)$$

$$\text{NADPH_production}(j, S_1, N_t) = \frac{j}{2} \cdot \frac{S_1}{N_t} \quad (26)$$

$$\text{NADPH_production}(j, S_1, N_t) = \frac{j}{2} \cdot \frac{S_1}{N_t} \quad (27)$$

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

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:

$$\frac{d}{dt} \text{RuBP} = 0 \quad (28)$$

9.2 Species PGA

Name PGA

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

This species takes part in three reactions (as a reactant in `PGA_cons` and as a product in `PGA_prod_Vc`, `PGA_prod_Vo`).

$$\frac{d}{dt} \text{PGA} = 2 v_1 + 1.5 v_2 - v_3 \quad (29)$$

9.3 Species NADPH

Name NADPH

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

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`).

$$\frac{d}{dt} \text{NADPH} = v_4 - 2 v_1 - 2 v_2 \quad (30)$$

9.4 Species CO2

Name CO2

Notes [Pa]

Initial concentration 35 mmol · l⁻¹

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

$$\frac{d}{dt} \text{CO}_2 = 0 \quad (31)$$

9.5 Species O2

Name O2

Notes [kPa]

Initial concentration 21 mmol · l⁻¹

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

$$\frac{d}{dt} \text{O}_2 = 0 \quad (32)$$

9.6 Species NADP

Name NADP

Initial concentration 0.29 mmol · 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

SBO:0000196 concentration of an entity pool: The amount of an entity per unit of volume.

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