SBML Model Report

Model name: "Rovers1995_Photsynthetic_Oscillations"

May 5, 2016

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by Rainer Machne[1] at January sixth 2011 at 11:40 p. m. and last time modified at April eighth 2016 at 4:53 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	6
events	0	constraints	0
reactions	4	function definitions	0
global parameters	6	unit definitions	8
rules	2	initial assignments	0

Model Notes

This is the model described in the article:
Photosynthetic oscillations and the interdependence of photophosphorylation and electron transport as studied by a mathematical model.
Rovers W, Giersch C. Biosystems. 1995;35(1):63-73. PMID: 7772723
Abstract:

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A simple mathematical model of photosynthetic carbon metabolism as driven by ATP and NADPH has been formulated to analyse photosynthetic oscillations. Two essential assumptions of this model are: (i) reduction of 3-phosphoglycerate to triosephosphate in the Clavin cycle is limited by ATP, not by NADPH, and (ii) photophosphorylation is affected by the availability of both ADP and NADP, while electron transport is limited by NADP only. The model produces oscillations of observed damping and period in ATP and NADP concentrations which are about 180 degrees out of phase, while three alternative proposals regarding coupling of electron transport and photophosphorylation do not produce oscillatory model solutions. The phases of ATP and NADPH are in reasonable agreement with the available experimental data. The model (which assumes that redox control of photophosphorylation is part of the oscillatory mechanism) is compared with an alternative proposal (that oscillations are due to interdependence of turnover of adenylates and Calvin cycle intermediates). From the similarity of the mathematical structures of both models it is inviting to speculate that both models are partial aspects of the oscillatory mechanism.

2 Unit Definitions

This is an overview of eight unit definitions.

2.1 Unit `substance`

Name mmole

Definition mmol

2.2 Unit `mM`

Name mM

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

2.3 Unit per_mM_per_s

Name per_mM_per_s

Definition $s^{-1} \cdot mmol^{-1} \cdot l$

2.4 Unit per_s

Name per_s

Definition s^{-1}

2.5 Unit volume

Name volume

Definition l

2.6 Unit area

Name area

Definition m^2

2.7 Unit length

Name length

Definition m

2.8 Unit time

Name 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
c		0000290	3	1	litre	☑	

3.1 Compartment c

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

SBO:0000290 physical compartment

4 Species

This model contains six 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
NADPH	NADPH	c	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☐
ADP	ADP	c	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☑
ATP	ATP	c	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☐
X	X	c	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☐
Y	Y	c	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑	☑
NADP	NADP_super_+	c	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☑

5 Parameters

This model contains six global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1		0000035	0.123	s^{-1}	☑
k2		0000035	0.625	s^{-1}	☑
k3		0000036	0.300	$s^{-1} \cdot mmol^{-1} \cdot l$	☑
k4		0000035	0.614	s^{-1}	☑
N0		0000472	1.200	$mmol \cdot l^{-1}$	☑
A0		0000472	2.500	$mmol \cdot l^{-1}$	☑

6 Rules

This is an overview of two rules.

6.1 Rule NADP

Rule NADP has the SBO reference 0000064 and is an assignment rule for species NADP:

$$NADP = N0 - [NADPH] \tag{1}$$

Derived unit $mmol \cdot l^{-1}$

6.2 Rule ADP

Rule ADP has the SBO reference 0000064 and is an assignment rule for species ADP:

$$ADP = A0 - [ATP] \tag{2}$$

Derived unit $mmol \cdot l^{-1}$

7 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	v4	v4	$\mathrm{NADP} \longrightarrow \mathrm{NADPH}$	0000202
2	v3	v3	$2\,\mathrm{ADP} \xrightarrow{\mathrm{NADP}} 2\,\mathrm{ATP}$	0000216
3	v2	v2	$\mathrm{Y} + \mathrm{NADPH} + \mathrm{ATP} \longrightarrow \mathrm{X} + \mathrm{ADP} + \mathrm{NADP}$	0000182
4	v1	v1	$\mathrm{X} + \mathrm{ATP} \longrightarrow \mathrm{Y} + \mathrm{ADP}$	0000216

7.1 Reaction v4

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

Name v4

SBO:0000202 reduction

Reaction equation

$$\mathrm{NADP} \longrightarrow \mathrm{NADPH} \tag{3}$$

Reactant

Table 6: Properties of each reactant.

Id	Name	SBO
NADP	NADP_super_+	0000010

Product

Table 7: Properties of each product.

Id	Name	SBO
NADPH	NADPH	0000011

Kinetic Law

SBO:0000049 mass action rate law for first order irreversible reactions, continuous scheme

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{mmol}$

$$v_1 = \mathrm{vol}\,(\mathrm{c}) \cdot \mathrm{k4} \cdot [\mathrm{NADP}] \tag{4}$$

7.2 Reaction v3

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

Name v3

SBO:0000216 phosphorylation

Reaction equation

$$2\,\mathrm{ADP} \xrightarrow{\mathrm{NADP}} 2\,\mathrm{ATP} \tag{5}$$

Reactant

Table 8: Properties of each reactant.

Id	Name	SBO
ADP	ADP	0000010

Modifier

Table 9: Properties of each modifier.

Id	Name	SBO
NADP	NADP_super_+	0000461

Product

Table 10: Properties of each product.

Id	Name	SBO
ATP	ATP	0000011

Kinetic Law

SBO:0000054 mass action rate law for second order irreversible reactions, two reactants, continuous scheme

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{mmol}$

$$v_2 = \mathrm{vol}\,(\mathrm{c}) \cdot \mathrm{k3} \cdot [\mathrm{ADP}] \cdot [\mathrm{NADP}] \tag{6}$$

7.3 Reaction v2

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

Name v2

SBO:0000182 conversion

Reaction equation

$$\mathrm{Y} + \mathrm{NADPH} + \mathrm{ATP} \longrightarrow \mathrm{X} + \mathrm{ADP} + \mathrm{NADP} \tag{7}$$

Reactants

Table 11: Properties of each reactant.

Id	Name	SBO
Y	Y	0000010
NADPH	NADPH	0000010
ATP	ATP	0000010

Products

Table 12: Properties of each product.

Id	Name	SBO
X	X	0000011
ADP	ADP	0000011
NADP	NADP_super_+	0000011

Kinetic Law

SBO:0000049 mass action rate law for first order irreversible reactions, continuous scheme

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{mmol}$

$$v_3 = \mathrm{vol}(\mathrm{c}) \cdot \mathrm{k2} \cdot [\mathrm{ATP}] \tag{8}$$

7.4 Reaction v1

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

Name v1

SBO:0000216 phosphorylation

Reaction equation

$$\mathrm{X} + \mathrm{ATP} \longrightarrow \mathrm{Y} + \mathrm{ADP} \tag{9}$$

Reactants

Table 13: Properties of each reactant.

Id	Name	SBO
X	X	0000010
ATP	ATP	0000010

Products

Table 14: Properties of each product.

Id	Name	SBO
Y	Y	0000011
ADP	ADP	0000011

Kinetic Law

SBO:0000049 mass action rate law for first order irreversible reactions, continuous scheme

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{mmol}$

$$v_4 = \mathrm{vol}\,(\mathrm{c}) \cdot \mathrm{k1} \cdot [\mathrm{X}] \tag{10}$$

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.

8.1 Species NADPH

Name NADPH

SBO:0000247 simple chemical

Initial concentration $0.7\ \mathrm{mmol} \cdot \mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in v2 and as a product in v4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{NADPH} = v_1 - v_3 \tag{11}$$

8.2 Species ADP

Name ADP

SBO:0000247 simple chemical

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

Involved in rule ADP

This species takes part in three reactions (as a reactant in v3 and as a product in v2, v1). Not these but one rule determines the species' quantity because this species is on the boundary of the reaction system.

8.3 Species ATP

Name ATP

SBO:0000247 simple chemical

Initial concentration $0.5\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in three reactions (as a reactant in v2, v1 and as a product in v3).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ATP} = 2v_2 - v_3 - v_4 \tag{12}$$

8.4 Species X

Name X

SBO:0000247 simple chemical

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

This species takes part in two reactions (as a reactant in v1 and as a product in v2).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{X} = v_3 - v_4 \tag{13}$$

8.5 Species Y

Name Y

SBO:0000247 simple chemical

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

This species takes part in two reactions (as a reactant in v2 and as a product in v1), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Y} = 0 \tag{14}$$

8.6 Species NADP

Name NADP_super_+

SBO:0000247 simple chemical

Initial concentration $0.5\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

Involved in rule NADP

This species takes part in three reactions (as a reactant in v4 and as a product in v2 and as a modifier in v3). Not these 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:0000010 reactant: Substance consumed by a chemical reaction. Reactants react with each other to form the products of a chemical reaction. In a chemical equation the Reactants are the elements or compounds on the left hand side of the reaction equation. A reactant can be consumed and produced by the same reaction, its global quantity remaining unchanged

SBO:0000011 product: Substance that is produced in a reaction. In a chemical equation the Products are the elements or compounds on the right hand side of the reaction equation. A product can be produced and consumed by the same reaction, its global quantity remaining unchanged

SBO:0000035 forward unimolecular rate constant, continuous case: Numerical parameter that quantifies the forward velocity of a chemical reaction involving only one reactant. This parameter encompasses all the contributions to the velocity except the quantity of the reactant. It is to be used in a reaction modelled using a continuous framework

SBO:0000036 forward bimolecular rate constant, continuous case: Numerical parameter that quantifies the forward velocity of a chemical reaction involving two reactants. This parameter encompasses all the contributions to the velocity except the quantity of the reactants. It is to be used in a reaction modelled using a continuous framework

SBO:0000049 mass action rate law for first order irreversible reactions, continuous scheme: Reaction scheme where the products are created from the reactants and the change of a product quantity is proportional to the product of reactant activities. The reaction scheme does not include any reverse process that creates the reactants from the products. The change of a product quantity is proportional to the quantity of one reactant. It is to be used in a reaction modelled using a continuous framework.

SBO:0000054 mass action rate law for second order irreversible reactions, two reactants, continuous scheme: Reaction scheme where the products are created from the reactants and the change of a product quantity is proportional to the product of reactant activities. The reaction scheme does not include any reverse process that creates the reactants from the products. The change of a product quantity is proportional to the product of two reactant quantities. It is to be used in a reaction modelled using a continuous framework.

SBO:0000064 mathematical expression: Formal representation of a calculus linking parameters and variables of a model

SBO:0000182 conversion: Biochemical reaction that results in the modification of some covalent bonds

SBO:0000202 reduction: Chemical process in which a molecular entity gain electrons

SBO:0000216 phosphorylation: Addition of a phosphate group (-H2PO4) to a chemical entity

SBO:0000247 simple chemical: Simple, non-repetitive chemical entity

SBO:0000290 physical compartment: Specific location of space, that can be bounded or not. A physical compartment can have 1, 2 or 3 dimensions

SBO:0000461 essential activator: A substance that is absolutely required for occurrence and stimulation of a reaction

SBO:0000472 molar concentration of an entity: Molarity, or molar concentration, denotes the number of moles of a given substance per litre of solution. The unit of measure of molarity is mol/L, molar, or the capital letter M as an abbreviated form

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