SBML Model Report

Model name: "Valero2006_Adenine_TernaryCycle"

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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 two authors: Vijayalakshmi Chelliah[1] and Edelmira Valero[2] at August 19th 2009 at 4:30 p. m. and last time modified at March nineth 2012 at 11:40 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	1
species types	0	species	6
events	0	constraints	0
reactions	4	function definitions	0
global parameters	9	unit definitions	0
rules	0	initial assignments	0

Model Notes

This a model from the article:
A kinetic study of a ternary cycle between adenine nucleotides.
Valero E, Varn R, Garca-Carmona F FEBS J. [2006 Aug;273(15):3598-613 16884499 ,
Abstract:

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In the present paper, a kinetic study is made of the behavior of a moiety-conserved ternary cycle between the adenine nucleotides. The system contains the enzymes S-acetyl coenzyme A synthetase, adenylate kinase and pyruvate kinase, and converts ATP into AMP, then into ADP and finally back to ATP. L-Lactate dehydrogenase is added to the system to enable continuous monitoring of the progress of the reaction. The cycle cannot work when the only recycling substrate in the reaction medium is AMP. A mathematical model is proposed whose kinetic behavior has been analyzed both numerically by integration of the nonlinear differential equations describing the kinetics of the reactions involved, and analytically under steady-state conditions, with good agreement with the experimental results being obtained. The data obtained showed that there is a threshold value of the S-acetyl coenzyme A synthetase/adenylate kinase ratio, above which the cycle stops because all the recycling substrate has been accumulated as AMP, never reaching the steady state. In addition, the concept of adenylate energy charge has been applied to the system, obtaining the enabled values of the rate constants for a fixed adenylate energy charge value and vice versa.

2 Unit Definitions

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

2.1 Unit `substance`

Notes Mole is the predefined SBML unit for `substance`.

Definition mol

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
`compartment`	compartment		3	1	litre	☑	

3.1 Compartment `compartment`

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

Name compartment

4 Species

This model contains six species. The boundary condition of one of these species is set to `true` so that this 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
ATP	ATP	compartment	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☐
AMP	AMP	compartment	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☐
ADP	ADP	compartment	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☐
Pyr	Pyr	compartment	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☐
NADH	NADH	compartment	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☐
Lac	Lac	compartment	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☑	☑

5 Parameters

This model contains nine global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vmapp1	Vmapp1		2.3		☑
Kmapp1	Kmapp1		700.0		☑
Vm2	Vm2		170.0		☑
Km2ATP	Km2ATP		25.0		☑
Km2AMP	Km2AMP		110.0		☑
K	K		71000.0		☑
Vmapp3	Vmapp3		65.0		☑
Kmapp3	Kmapp3		260.0		☑
k4	k4		5.0		☑

6 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	v1	v1	$\mathrm{ATP} \rightleftharpoons \mathrm{AMP}$	
2	v2	v2	$\mathrm{ATP} + \mathrm{AMP} \rightleftharpoons 2\,\mathrm{ADP}$	
3	v3	v3	$\mathrm{ADP} \rightleftharpoons \mathrm{ATP} + \mathrm{Pyr}$	
4	v4	v4	$\mathrm{Pyr} + \mathrm{NADH} \rightleftharpoons \mathrm{Lac}$	

6.1 Reaction v1

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

Name v1

Reaction equation

$$\mathrm{ATP} \rightleftharpoons \mathrm{AMP} \tag{1}$$

Reactant

Table 6: Properties of each reactant.

Id	Name	SBO
ATP	ATP	

Product

Table 7: Properties of each product.

Id	Name	SBO
AMP	AMP	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \frac{\mathrm{Vmapp1} \cdot [\mathrm{ATP}]}{\mathrm{Kmapp1} + [\mathrm{ATP}]} \tag{2}$$

6.2 Reaction v2

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

Name v2

Reaction equation

$$\mathrm{ATP} + \mathrm{AMP} \rightleftharpoons 2\,\mathrm{ADP} \tag{3}$$

Reactants

Table 8: Properties of each reactant.

Id	Name	SBO
ATP	ATP	
AMP	AMP	

Product

Table 9: Properties of each product.

Id	Name	SBO
ADP	ADP	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \frac{\mathrm{Vm2} \cdot [\mathrm{ATP}] \cdot [\mathrm{AMP}]}{\mathrm{K} + \mathrm{Km2ATP} \cdot [\mathrm{AMP}] + \mathrm{Km2AMP} \cdot [\mathrm{ATP}] + [\mathrm{ATP}] \cdot [\mathrm{AMP}]} \tag{4}$$

6.3 Reaction v3

This is a reversible reaction of one reactant forming two products.

Name v3

Reaction equation

$$\mathrm{ADP} \rightleftharpoons \mathrm{ATP} + \mathrm{Pyr} \tag{5}$$

Reactant

Table 10: Properties of each reactant.

Id	Name	SBO
ADP	ADP	

Products

Table 11: Properties of each product.

Id	Name	SBO
ATP	ATP	
Pyr	Pyr	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \frac{\text{Vmapp3} \cdot [\text{ADP}]}{\text{Kmapp3} + [\text{ADP}]} \tag{6}$$

6.4 Reaction v4

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

Name v4

Reaction equation

$$\text{Pyr} + \text{NADH} \rightleftharpoons \text{Lac} \tag{7}$$

Reactants

Table 12: Properties of each reactant.

Id	Name	SBO
Pyr	Pyr	
NADH	NADH	

Product

Table 13: Properties of each product.

Id	Name	SBO
Lac	Lac	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \text{k4} \cdot [\text{Pyr}] \tag{8}$$

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 `ATP`

Name ATP

SBO:0000247 simple chemical

Initial concentration $16.3\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ATP} = v_3 - v_1 - v_2 \tag{9}$$

7.2 Species `AMP`

Name AMP

SBO:0000247 simple chemical

Initial concentration $0\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{AMP} = v_1 - v_2 \tag{10}$$

7.3 Species `ADP`

Name ADP

SBO:0000247 simple chemical

Initial concentration $0\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in `v3` and as a product in `v2`).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ADP} = 2\,v_2 - v_3 \tag{11}$$

7.4 Species Pyr

Name Pyr

SBO:0000014 enzyme

Initial concentration $0\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in v4 and as a product in v3).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Pyr} = v_3 - v_4 \tag{12}$$

7.5 Species NADH

Name NADH

SBO:0000247 simple chemical

Initial concentration $256\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in one reaction (as a reactant in v4).

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

7.6 Species Lac

Name Lac

SBO:0000014 enzyme

Initial concentration $0\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in one reaction (as a product in v4), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

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

A Glossary of Systems Biology Ontology Terms

SBO:0000014 enzyme: A protein that catalyzes a chemical reaction. The word comes from en “a” or“i”) and simo “leave” or“yeas”)

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

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