SBML Model Report

Model name: "Nazaret2009_TCA_RC_ATP"

May 6, 2016

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 Kieran Smallbone[2] at September tenth 2009 at no o' clock in the morning. and last time modified at January 22nd 2010 at 3:30 p. m. Table 1 shows 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	2
species types	0	species	14
events	0	constraints	0
reactions	12	function definitions	0
global parameters	22	unit definitions	14
rules	9	initial assignments	1

Model Notes

This a model from the article:
Mitochondrial energetic metabolism: a simplified model of TCA cycle with ATP production.
Nazaret C, Heiske M, Thurley K, Mazat JP J. Theor. Biol. 2009 Jun;258(3):455-64 19007794 ,
Abstract:
Mitochondria play a central role in cellular energetic metabolism. The essential parts of this

[1]EMBL-EBI, viji@ebi.ac.uk
[2]University of Manchester, kieran.smallbone@manchester.ac.uk

metabolism are the tricarboxylic acid (TCA) cycle, the respiratory chain and the adenosine triphosphate (ATP) synthesis machinery. Here a simplified model of these three metabolic components with a limited set of differential equations is presented. The existence of a steady state is demonstrated and results of numerical simulations are presented. The relevance of a simple model to represent actual in vivo behavior is discussed.

2 Unit Definitions

This is an overview of 18 unit definitions of which four are predefined by SBML and not mentioned in the model.

2.1 Unit substance

Definition mmol

2.2 Unit C_per_mol

Name coulomb per mole

Definition $\mathrm{daC} \cdot \mathrm{damol}^{-1}$

2.3 Unit mJ_per_mol_per_K

Name milliJoule per mole per Kelvin

Definition $\mathrm{mJ} \cdot \mathrm{damol}^{-1} \cdot \mathrm{daK}^{-1}$

2.4 Unit mJ_per_mol

Name milliJoules per mole

Definition $\mathrm{mJ} \cdot \mathrm{damol}^{-1}$

2.5 Unit mM

Name millimolar

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

2.6 Unit mM_per_mV

Name millimolar per millivolt

Definition $\mathrm{mmol} \cdot \mathrm{dal}^{-1} \cdot \mathrm{mV}^{-1}$

2.7 Unit mM_per_s

Name millimolar per second

Definition $\mathrm{mmol} \cdot \mathrm{dal}^{-1} \cdot \mathrm{das}^{-1}$

2.8 Unit mM_per_s_per_mV

Name millimolar per second per millivolt

Definition $\mathrm{mmol} \cdot \mathrm{dal}^{-1} \cdot \mathrm{das}^{-1} \cdot \mathrm{mV}^{-1}$

2.9 Unit mV

Name millivolt

Definition mV

2.10 Unit per_mM

Name per mM

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

2.11 Unit per_mM_per_s

Name per millimolar per second

Definition $\mathrm{mmol}^{-1} \cdot \mathrm{dal} \cdot \mathrm{das}^{-1}$

2.12 Unit per_mM_squared_per_s

Name per millimolar squared per second

Definition $\mathrm{mmol}^{-2} \cdot \mathrm{dal}^{2} \cdot \mathrm{das}^{-1}$

2.13 Unit per_mV

Name per millivolt

Definition mV^{-1}

2.14 Unit per_s

Name per second

Definition das^{-1}

2.15 Unit volume

Notes Litre is the predefined SBML unit for volume.

Definition l

2.16 Unit area

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

Definition m^2

2.17 Unit length

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

Definition m

2.18 Unit time

Notes Second is the predefined SBML unit for time.

Definition s

3 Compartments

This model contains two compartments.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
cytoplasm	cytoplasm	0000290	3	1	litre	☑	
mitochondrion	mitochondrial matrix	0000290	3	1	litre	☑	

3.1 Compartment cytoplasm

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

Name cytoplasm

SBO:0000290 physical compartment

3.2 Compartment mitochondrion

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

Name mitochondrial matrix

SBO:0000290 physical compartment

4 Species

This model contains 14 species. The boundary condition of seven 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
ADP	ADP	mitochondrion	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☑
ATP	ATP	mitochondrion	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☐
H	H+	mitochondrion	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑	☑
He	H+	cytoplasm	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑	☑
NAD	NAD(+)	mitochondrion	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☐
NADH	NADH	mitochondrion	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☑
AcCoA	acetyl-CoA	mitochondrion	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☐
KG	alpha-ketoglutarate	mitochondrion	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☐
Cit	citrate	mitochondrion	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☐
OAA	oxaloacetate	mitochondrion	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☐
O2	oxygen	mitochondrion	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑	☑
iP	phosphate	mitochondrion	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑	☑
Pyr	pyruvate	mitochondrion	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☐
H2O	water	mitochondrion	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☑	☑

5 Parameters

This model contains 22 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
ATPcrit			0.000	$\mathrm{mmol \cdot dal^{-1}}$	⊟
At			4.160	$\mathrm{mmol \cdot dal^{-1}}$	☑
C			$6.75 \cdot 10^{-6}$	$\mathrm{mmol \cdot dal^{-1} \cdot mV^{-1}}$	☑
DeltaGtransport			0.000	$\mathrm{mJ \cdot damol^{-1}}$	⊟
DeltaPsi			0.000	mV	⊟
DeltaPsim			150.000	mV	☑
F	Faraday constant		96485.000	$\mathrm{daC \cdot damol^{-1}}$	☑
JANT			0.000	$\mathrm{mmol \cdot dal^{-1} \cdot das^{-1}}$	⊟
JATP			0.000	$\mathrm{mmol \cdot dal^{-1} \cdot das^{-1}}$	⊟
Jleak			0.000	$\mathrm{mmol \cdot dal^{-1} \cdot das^{-1}}$	⊟
Jresp			0.000	$\mathrm{mmol \cdot dal^{-1} \cdot das^{-1}}$	⊟
K			2.000	$\mathrm{mmol \cdot dal^{-1}}$	☑
Kapp			$4.4 \cdot 10^{-9}$	$\mathrm{mmol^{-1} \cdot dal}$	☑
Nt			1.070	$\mathrm{mmol \cdot dal^{-1}}$	☑
R	gas constant		8314.000	$\mathrm{mJ \cdot damol^{-1} \cdot daK^{-1}}$	☑
T	absolute temperature		298.000	K	☑
a			0.100	$\mathrm{mV^{-1}}$	☑
b			0.004	$\mathrm{mmol^{-1} \cdot dal}$	☑
kANT			0.054	$\mathrm{das^{-1}}$	☑
kATP			131.900	$\mathrm{mmol \cdot dal^{-1} \cdot das^{-1}}$	☑
kleak			$4.26 \cdot 10^{-4}$	$\mathrm{mmol \cdot dal^{-1} \cdot das^{-1} \cdot mV^{-1}}$	☑
kresp			2.500	$\mathrm{mmol \cdot dal^{-1} \cdot das^{-1}}$	☑

6 Initialassignment

This is an overview of one initialassignment.

6.1 Initialassignment DeltaPsi

Derived unit contains undeclared units

Math 150

7 Rules

This is an overview of nine rules.

7.1 Rule JANT

Rule JANT is an assignment rule for parameter JANT:

$$\mathrm{JANT} = \mathrm{kANT} \cdot [\mathrm{ATP}] \tag{1}$$

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

7.2 Rule Jleak

Rule Jleak is an assignment rule for parameter Jleak:

$$\mathrm{Jleak} = \mathrm{kleak} \cdot \mathrm{DeltaPsi} \tag{2}$$

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

7.3 Rule DeltaPsi

Rule DeltaPsi is a rate rule for parameter DeltaPsi:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{DeltaPsi} = \frac{10 \cdot \mathrm{Jresp} - 3 \cdot \mathrm{JATP} - \mathrm{Jleak} - \mathrm{JANT}}{\mathrm{C}} \tag{3}$$

7.4 Rule Jresp

Rule Jresp is an assignment rule for parameter Jresp:

$$\mathrm{Jresp} = \frac{\mathrm{kresp} \cdot \frac{\mathrm{Nt} - [\mathrm{NAD}]}{\mathrm{K} + \mathrm{Nt} - [\mathrm{NAD}]}}{1 + \exp\left(\mathrm{a} \cdot (\mathrm{DeltaPsi} - \mathrm{DeltaPsim})\right)} \tag{4}$$

7.5 Rule JATP

Rule JATP is an assignment rule for parameter JATP:

$$\mathrm{JATP} = \mathrm{kATP} \cdot \left(\frac{2}{1 + \exp\left(\mathrm{b} \cdot ([\mathrm{ATP}] - \mathrm{ATPcrit})\right)} - 1 \right) \tag{5}$$

7.6 Rule ATPcrit

Rule ATPcrit is an assignment rule for parameter ATPcrit:

$$\mathrm{ATPcrit} = \frac{\mathrm{At}}{1 + \frac{\exp\left(\frac{-3 \cdot \mathrm{DeltaGtransport}}{\mathrm{R} \cdot \mathrm{T}}\right)}{\mathrm{Kapp} \cdot [\mathrm{iP}]}} \tag{6}$$

7.7 Rule DeltaGtransport

Rule DeltaGtransport is an assignment rule for parameter DeltaGtransport:

$$\text{DeltaGtransport} = 1.2 \cdot \text{F} \cdot \text{DeltaPsi} \tag{7}$$

7.8 Rule ADP

Rule ADP is an assignment rule for species ADP:

$$\text{ADP} = \text{At} - [\text{ATP}] \tag{8}$$

Derived unit $\text{mmol} \cdot \text{dal}^{-1}$

7.9 Rule NADH

Rule NADH is an assignment rule for species NADH:

$$\text{NADH} = \text{Nt} - [\text{NAD}] \tag{9}$$

Derived unit $\text{mmol} \cdot \text{dal}^{-1}$

8 Reactions

This model contains twelve 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	$\emptyset \longrightarrow \mathrm{Pyr}$	0000185
2	v2	v2	$\mathrm{Pyr} + \mathrm{NAD} \longrightarrow \mathrm{AcCoA} + \mathrm{NADH}$	0000399
3	v3	v3	$\mathrm{OAA} + \mathrm{AcCoA} \longrightarrow \mathrm{Cit}$	0000210
4	v4	v4	$\mathrm{Cit} + \mathrm{NAD} \longrightarrow \mathrm{KG} + \mathrm{NADH}$	0000399
5	v5	v5	$\mathrm{KG} + \mathrm{ADP} + 2\,\mathrm{NAD} \longrightarrow \mathrm{OAA} + \mathrm{ATP} + 2\,\mathrm{NADH}$	0000399
6	v6	v6	$\mathrm{OAA} \rightleftharpoons \mathrm{KG}$	0000403
7	v7	v7	$\mathrm{Pyr} + \mathrm{ATP} \longrightarrow \mathrm{OAA} + \mathrm{ADP}$	0000210
8	v8	v8	$\mathrm{OAA} \longrightarrow \emptyset$	0000185
9	vresp	vresp	$\mathrm{NADH} + 0 \cdot 5\,\mathrm{O2} + 11\,\mathrm{H} \longrightarrow \mathrm{NAD} + \mathrm{H2O} + 10\,\mathrm{He}$	0000201
10	vATP	vATP	$\mathrm{ADP} + \mathrm{iP} + 3\,\mathrm{He} \rightleftharpoons \mathrm{ATP} + \mathrm{H2O} + 3\,\mathrm{H}$	0000216
11	vANT	vANT	$\mathrm{ATP} \longrightarrow \mathrm{ADP}$	0000330
12	vleak	vleak	$\mathrm{He} \longrightarrow \mathrm{H}$	0000185

8.1 Reaction v1

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

Name v1

SBO:0000185 transport reaction

Reaction equation

$$\emptyset \longrightarrow \mathrm{Pyr} \tag{10}$$

Product

Table 6: Properties of each product.

Id	Name	SBO
Pyr	pyruvate	

Kinetic Law

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

$$v_1 = \mathrm{vol}\,(\mathrm{mitochondrion}) \cdot \mathrm{k1} \tag{11}$$

Table 7: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1			0.038	$\mathrm{mmol} \cdot \mathrm{dal}^{-1} \cdot \mathrm{das}^{-1}$	☑

8.2 Reaction v2

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

Name v2

SBO:0000399 decarboxylation

Reaction equation

$$\mathrm{Pyr} + \mathrm{NAD} \longrightarrow \mathrm{AcCoA} + \mathrm{NADH} \tag{12}$$

Reactants

Table 8: Properties of each reactant.

Id	Name	SBO
Pyr	pyruvate	
NAD	NAD(+)	

Products

Table 9: Properties of each product.

Id	Name	SBO
AcCoA	acetyl-CoA	
NADH	NADH	

Kinetic Law

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

$$v_2 = \mathrm{vol}\,(\mathrm{mitochondrion}) \cdot \mathrm{k2} \cdot [\mathrm{Pyr}] \cdot [\mathrm{NAD}] \tag{13}$$

Table 10: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k2			0.152	$\mathrm{mmol}^{-1} \cdot \mathrm{dal} \cdot \mathrm{das}^{-1}$	☑

8.3 Reaction v3

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

Name v3

SBO:0000210 addition of a chemical group

Reaction equation

$$\mathrm{OAA} + \mathrm{AcCoA} \longrightarrow \mathrm{Cit} \tag{14}$$

Reactants

Table 11: Properties of each reactant.

Id	Name	SBO
OAA	oxaloacetate	
AcCoA	acetyl-CoA	

Product

Table 12: Properties of each product.

Id	Name	SBO
Cit	citrate	

Kinetic Law

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

$$v_3 = \mathrm{vol}\,(\mathrm{mitochondrion}) \cdot \mathrm{k3} \cdot [\mathrm{OAA}] \cdot [\mathrm{AcCoA}] \tag{15}$$

Table 13: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k3			57.142	$\mathrm{mmol}^{-1} \cdot \mathrm{dal} \cdot \mathrm{das}^{-1}$	☑

8.4 Reaction v4

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

Name v4

SBO:0000399 decarboxylation

Reaction equation

$$\mathrm{Cit} + \mathrm{NAD} \longrightarrow \mathrm{KG} + \mathrm{NADH} \tag{16}$$

Reactants

Table 14: Properties of each reactant.

Id	Name	SBO
Cit	citrate	

Id	Name	SBO
NAD	NAD(+)	

Products

Table 15: Properties of each product.

Id	Name	SBO
KG	alpha-ketoglutarate	
NADH	NADH	

Kinetic Law

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

$$v_4 = \mathrm{vol}\,(\mathrm{mitochondrion}) \cdot \mathrm{k4} \cdot [\mathrm{Cit}] \cdot [\mathrm{NAD}] \tag{17}$$

Table 16: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k4			0.053	$\mathrm{mmol}^{-1} \cdot \mathrm{dal} \cdot \mathrm{das}^{-1}$	☑

8.5 Reaction v5

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

Name v5

SBO:0000399 decarboxylation

Reaction equation

$$\mathrm{KG} + \mathrm{ADP} + 2\,\mathrm{NAD} \longrightarrow \mathrm{OAA} + \mathrm{ATP} + 2\,\mathrm{NADH} \tag{18}$$

Reactants

Table 17: Properties of each reactant.

Id	Name	SBO
KG	alpha-ketoglutarate	
ADP	ADP	

Id	Name	SBO
NAD	NAD(+)	

Products

Table 18: Properties of each product.

Id	Name	SBO
OAA	oxaloacetate	
ATP	ATP	
NADH	NADH	

Kinetic Law

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

$$v_5 = \mathrm{vol}\,(\mathrm{mitochondrion}) \cdot \mathrm{k5} \cdot [\mathrm{KG}] \cdot [\mathrm{NAD}] \cdot (\mathrm{At} - [\mathrm{ATP}]) \tag{19}$$

Table 19: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k5			0.082	$\mathrm{mmol}^{-2} \cdot \mathrm{dal}^2 \cdot \mathrm{das}^{-1}$	☑

8.6 Reaction v6

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

Name v6

SBO:0000403 transamination

Reaction equation

$$\mathrm{OAA} \rightleftharpoons \mathrm{KG} \tag{20}$$

Reactant

Table 20: Properties of each reactant.

Id	Name	SBO
OAA	oxaloacetate	

Product

Table 21: Properties of each product.

Id	Name	SBO
KG	alpha-ketoglutarate	

Kinetic Law

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

$$v_6 = \mathrm{vol}\,(\mathrm{mitochondrion}) \cdot \mathrm{k6} \cdot \left([\mathrm{OAA}] - \frac{[\mathrm{KG}]}{\mathrm{Keq}} \right) \tag{21}$$

Table 22: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k6			0.003	das^{-1}	☑
Keq		0000281	0.398	dimensionless	☑

8.7 Reaction v7

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

Name v7

SBO:0000210 addition of a chemical group

Reaction equation

$$\mathrm{Pyr} + \mathrm{ATP} \longrightarrow \mathrm{OAA} + \mathrm{ADP} \tag{22}$$

Reactants

Table 23: Properties of each reactant.

Id	Name	SBO
Pyr	pyruvate	
ATP	ATP	

Products

Table 24: Properties of each product.

Id	Name	SBO
OAA	oxaloacetate	
ADP	ADP	

Kinetic Law

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

$$v_7 = \mathrm{vol}\,(\mathrm{mitochondrion}) \cdot \mathrm{k7} \cdot [\mathrm{Pyr}] \cdot [\mathrm{ATP}] \tag{23}$$

Table 25: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k7			0.04	$\mathrm{mmol}^{-1} \cdot \mathrm{dal} \cdot \mathrm{das}^{-1}$	☑

8.8 Reaction v8

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

Name v8

SBO:0000185 transport reaction

Reaction equation

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

Reactant

Table 26: Properties of each reactant.

Id	Name	SBO
OAA	oxaloacetate	

Kinetic Law

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

$$v_8 = \mathrm{vol}\,(\mathrm{mitochondrion}) \cdot \mathrm{k8} \cdot [\mathrm{OAA}] \tag{25}$$

Table 27: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k8			3.6	das^{-1}	☑

8.9 Reaction vresp

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

Name vresp

SBO:0000201 oxidation

Reaction equation

$$\mathrm{NADH} + 0{\cdot}5\,\mathrm{O2} + 11\,\mathrm{H} \longrightarrow \mathrm{NAD} + \mathrm{H2O} + 10\,\mathrm{He} \tag{26}$$

Reactants

Table 28: Properties of each reactant.

Id	Name	SBO
NADH	NADH	
O2	oxygen	
H	H+	

Products

Table 29: Properties of each product.

Id	Name	SBO
NAD	NAD(+)	
H2O	water	
He	H+	

Kinetic Law

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

$$v_9 = \mathrm{vol}\,(\mathrm{mitochondrion}) \cdot \mathrm{Jresp} \tag{27}$$

8.10 Reaction vATP

This is a reversible reaction of three reactants forming three products.

Name vATP

SBO:0000216 phosphorylation

Reaction equation

$$\mathrm{ADP} + \mathrm{iP} + 3\,\mathrm{He} \rightleftharpoons \mathrm{ATP} + \mathrm{H2O} + 3\,\mathrm{H} \tag{28}$$

Reactants

Table 30: Properties of each reactant.

Id	Name	SBO
ADP	ADP	
iP	phosphate	
He	H+	

Products

Table 31: Properties of each product.

Id	Name	SBO
ATP	ATP	
H2O	water	
H	H+	

Kinetic Law

Derived unit $\text{mmol} \cdot \text{das}^{-1}$

$$v_{10} = \text{vol}\,(\text{mitochondrion}) \cdot \text{JATP} \tag{29}$$

8.11 Reaction vANT

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

Name vANT

SBO:0000330 dephosphorylation

Reaction equation

$$\text{ATP} \longrightarrow \text{ADP} \tag{30}$$

Reactant

Table 32: Properties of each reactant.

Id	Name	SBO
ATP	ATP	

Product

Table 33: Properties of each product.

Id	Name	SBO
ADP	ADP	

Kinetic Law

Derived unit $\text{mmol} \cdot \text{das}^{-1}$

$$v_{11} = \text{vol}\,(\text{mitochondrion}) \cdot \text{JANT} \tag{31}$$

8.12 Reaction vleak

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

Name vleak

SBO:0000185 transport reaction

Reaction equation

$$\mathrm{He} \longrightarrow \mathrm{H} \tag{32}$$

Reactant

Table 34: Properties of each reactant.

Id	Name	SBO
He	H+	

Product

Table 35: Properties of each product.

Id	Name	SBO
H	H+	

Kinetic Law

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

$$v_{12} = \mathrm{vol}\,(\mathrm{mitochondrion}) \cdot \mathrm{Jleak} \tag{33}$$

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.

9.1 Species ADP

Name ADP

SBO:0000247 simple chemical

Involved in rule ADP

This species takes part in four reactions (as a reactant in v5, vATP and as a product in v7, vANT). Not these but one rule determines the species' quantity because this species is on the boundary of the reaction system.

9.2 Species ATP

Name ATP

SBO:0000247 simple chemical

Initial concentration $3.536\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in four reactions (as a reactant in v7, vANT and as a product in v5, vATP).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ATP} = v_5 + v_{10} - v_7 - v_{11} \tag{34}$$

9.3 Species H

Name H+

SBO:0000327 non-macromolecular ion

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{H} = 0 \tag{35}$$

9.4 Species He

Name H+

SBO:0000327 non-macromolecular ion

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{He} = 0 \tag{36}$$

9.5 Species NAD

Name NAD(+)

SBO:0000247 simple chemical

Initial concentration $0.856\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in four reactions (as a reactant in v2, v4, v5 and as a product in vresp).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{NAD} = v_9 - v_2 - v_4 - 2v_5 \tag{37}$$

9.6 Species NADH

Name NADH

SBO:0000247 simple chemical

Involved in rule NADH

This species takes part in four reactions (as a reactant in vresp and as a product in v2, v4, v5). Not these but one rule determines the species' quantity because this species is on the boundary of the reaction system.

9.7 Species AcCoA

Name acetyl-CoA

SBO:0000247 simple chemical

Initial concentration $0.063\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{AcCoA} = v_2 - v_3 \tag{38}$$

9.8 Species KG

Name alpha-ketoglutarate

SBO:0000247 simple chemical

Initial concentration $0.225\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in three reactions (as a reactant in v5 and as a product in v4, v6).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{KG} = v_4 + v_6 - v_5 \tag{39}$$

9.9 Species Cit

Name citrate

SBO:0000247 simple chemical

Initial concentration $0.44\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Cit} = v_3 - v_4 \tag{40}$$

9.10 Species OAA

Name oxaloacetate

SBO:0000247 simple chemical

Initial concentration $0.0050\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in five reactions (as a reactant in v3, v6, v8 and as a product in v5, v7).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{OAA} = v_5 + v_7 - v_3 - v_6 - v_8 \tag{41}$$

9.11 Species O2

Name oxygen

SBO:0000247 simple chemical

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{O2} = 0 \tag{42}$$

9.12 Species iP

Name phosphate

SBO:0000327 non-macromolecular ion

Initial concentration $2.44\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{iP} = 0 \tag{43}$$

9.13 Species Pyr

Name pyruvate

SBO:0000247 simple chemical

Initial concentration $0.154\ \mathrm{mmol}\cdot\mathrm{l}^{-1}$

This species takes part in three reactions (as a reactant in v2, v7 and as a product in v1).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Pyr} = v_1 - v_2 - v_7 \tag{44}$$

9.14 Species H2O

Name water

SBO:0000247 simple chemical

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{H2O} = 0 \tag{45}$$

A Glossary of Systems Biology Ontology Terms

SBO:0000185 transport reaction: Movement of a physical entity without modification of the structure of the entity

SBO:0000201 oxidation: Chemical process during which a molecular entity loses electrons

SBO:0000210 addition of a chemical group: Covalent reaction that results in the addition of a chemical group on a molecule

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

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

SBO:0000281 equilibrium constant: Quantity characterizing a chemical equilibrium in a chemical reaction, which is a useful tool to determine the concentration of various reactants or products in a system where chemical equilibrium occurs

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:0000327 non-macromolecular ion: Chemical entity having a net electric charge

SBO:0000330 dephosphorylation: Removal of a phosphate group (-H2PO4) from a chemical entity.

SBO:0000399 decarboxylation: A process in which a carboxyl group (COOH) is removed from a molecule as carbon dioxide

SBO:0000403 transamination: The transfer of an amino group between two molecules. Commonly in biology this is restricted to reactions between an amino acid and an alpha-keto carbonic acid, whereby the reacting amino acid is converted into an alpha-keto acid, and the alpha-keto acid reactant into an amino acid

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.

[a]Center for Bioinformatics Tübingen (ZBIT), Germany
[b]California Institute of Technology, Beckman Institute BNMC, Pasadena, United States
[c]European Bioinformatics Institute, Wellcome Trust Genome Campus, Hinxton, United Kingdom
[d]EML Research gGmbH, Heidelberg, Germany