SBML Model Report

Model name: "Bruggeman2005_AmmoniumAssimilation"

May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 3 format. This model was created by the following three authors: Lukas Endler[1], Vijayalakshmi Chelliah[2] and Frank Bruggeman[3] at November 28th 2008 at 5:24 p. m. and last time modified at August nineth 2012 at 4:34 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	22
events	0	constraints	0
reactions	16	function definitions	0
global parameters	98	unit definitions	2
rules	4	initial assignments	0

Model Notes

This a model from the article:
The multifarious short-term regulation of ammonium assimilation of Escherichia coli: dissection using an in silico replica.

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Bruggeman FJ, Boogerd FC, Westerhoff HV. FEBS J. 2005 Apr;272(8):1965-85. 15819889 ,
Abstract:
Ammonium assimilation in Escherichia coli is regulated through multiple mechanisms (metabolic, signal transduction leading to covalent modification, transcription, and translation), which (in-)directly affect the activities of its two ammonium-assimilating enzymes, i.e. glutamine synthetase (GS) and glutamate dehydrogenase (GDH). Much is known about the kinetic properties of the components of the regulatory network that these enzymes are part of, but the ways in which, and the extents to which the network leads to subtle and quasi-intelligent regulation are unappreciated. To determine whether our present knowledge of the interactions between and the kinetic properties of the components of this network is complete - to the extent that when integrated in a kinetic model it suffices to calculate observed physiological behaviour - we now construct a kinetic model of this network, based on all of the kinetic data on the components that is available in the literature. We use this model to analyse regulation of ammonium assimilation at various carbon statuses for cells that have adapted to low and high ammonium concentrations. We show how a sudden increase in ammonium availability brings about a rapid redirection of the ammonium assimilation flux from GS/glutamate synthase (GOGAT) to GDH. The extent of redistribution depends on the nitrogen and carbon status of the cell. We develop a method to quantify the relative importance of the various regulators in the network. We find the importance is shared among regulators. We confirm that the adenylylation state of GS is the major regulator but that a total of 40% of the regulation is mediated by ADP (22%), glutamate (10%), glutamine (7%) and ATP (1%). The total steady-state ammonium assimilation flux is remarkably robust against changes in the ammonium concentration, but the fluxes through GS and GDH are completely nonrobust. Gene expression of GOGAT above a threshold value makes expression of GS under ammonium-limited conditions, and of GDH under glucose-limited conditions, sufficient for ammonium assimilation.

This version of the model originates from JWS online . The original model can be retrieved here .

2 Unit Definitions

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

2.1 Unit `time`

Name mins

Definition 60 s

2.2 Unit `milliMolar`

Name mM

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

2.3 Unit `substance`

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

Definition mol

2.4 Unit `volume`

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

Definition l

2.5 Unit `area`

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

Definition m^2

2.6 Unit `length`

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

Definition m

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 22 species. The boundary condition of ten 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
PII	PII	compartment	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☐
UTP	UTP	compartment	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☑	☑
PIIUMP	PIIUMP	compartment	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☐
PPi	PPi	compartment	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☑	☑
GLN	GLN	compartment	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☐
PIIUMP2	PIIUMP2	compartment	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☐
PIIUMP3	PIIUMP3	compartment	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☐
UMP	UMP	compartment	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☑	☑
GS	GS	compartment	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☐
AMP	AMP	compartment	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☐
NH4	NH4	compartment	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☑	☑
KG	KG	compartment	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☑	☑
NADPH	NADPH	compartment	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☑	☑
GLU	GLU	compartment	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☐
NADP	NADP	compartment	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☑	☑
AZGLU	AZGLU	compartment	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☐
ATP	ATP	compartment	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☐
ADP	ADP	compartment	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☐
AZglu	AZglu	compartment	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☑	☑
AZGLN	AZGLN	compartment	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☐
AZgln	AZgln	compartment	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☑	☑

Id	Name	Compartment	Derived Unit	Constant	Boundary Condition
P_i	P_i	compartment	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	☑

5 Parameters

This model contains 98 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
UT	UT		$6 \cdot 10^{-4}$		☑
kcatut	kcatut		137.000		☑
Kglnut	Kglnut		0.070		☑
Kutipii	Kutipii		0.002		☑
Kutpii	Kutpii		0.003		☑
Kutpiiump	Kutpiiump		0.004		☑
Kututp	Kututp		0.040		☑
Kutippi	Kutippi		0.114		☑
UR	UR		$6 \cdot 10^{-4}$		☑
kcatur	kcatur		5.500		☑
Kurpiiump	Kurpiiump		0.002		☑
Kurump	Kurump		8.400		☑
Kglnur	Kglnur		0.070		☑
a1	a1		10^{-22}		☑
b1	b1		0.517		☑
c1	c1		0.597		☑
d1	d1		0.039		☑
Vad	Vad		0.500		☑
Kadpiikg	Kadpiikg		$1.052 \cdot 10^{-5}$		☑
Kadgln	Kadgln		0.971		☑
Kadgs	Kadgs		0.002		☑
e1	e1		10^{-22}		☑
f1	f1		2.766		☑
g1	g1		3.323		☑
h1	h1		0.215		☑
i1	i1		10^{-22}		☑
j1	j1		10^{-22}		☑
k1	k1		10^{-22}		☑
l1	l1		0.023		☑
m1	m1		0.882		☑
n1	n1		8.491		☑
o1	o1		0.879		☑
Vdead	Vdead		0.500		☑
Kdeadpiikg	Kdeadpiikg		$2.274 \cdot 10^{-6}$		☑
Kdeadgln	Kdeadgln		0.044		☑
Kdeadpiiu	Kdeadpiiu		$1.805 \cdot 10^{-5}$		☑
Kdeadgsa	Kdeadgsa		$2.015 \cdot 10^{-4}$		☑

Id	Name	SBO	Value	Unit	Constant
Vgdh	Vgdh		360.000		☑
Kgdhkg	Kgdhkg		0.320		☑
Kgdhnh	Kgdhnh		1.100		☑
Kgdhglu	Kgdhglu		10.000		☑
Kgdhnadph	Kgdhnadph		0.040		☑
Kgdhnadp	Kgdhnadp		0.042		☑
Keqgdh	Keqgdh		1290.000		☑
Kgdhazglu	Kgdhazglu		2.500		☑
Vgog	Vgog		85.000		☑
Kgoggln	Kgoggln		0.175		☑
Kgogkg	Kgogkg		0.007		☑
Kgognadph	Kgognadph		0.002		☑
Kgogglu	Kgogglu		11.000		☑
Kgognadp	Kgognadp		0.004		☑
Kgogaz	Kgogaz		0.650		☑
Vgs	Vgs		600.000		☑
aamp	aamp		10.000		☑
bamp	bamp		2.367		☑
camp	camp		0.101		☑
damp	damp		10.869		☑
n1amp	n1amp		1.146		☑
n2amp	n2amp		19.217		☑
Kgseq	Kgseq		460.000		☑
Kgsatp	Kgsatp		0.350		☑
Kgsglu	Kgsglu		4.100		☑
Kgsnh	Kgsnh		0.100		☑
Kgsadp	Kgsadp		0.059		☑
Kgspi	Kgspi		3.700		☑
Kgsgln	Kgsgln		5.650		☑
Keq	Keq		460.000	dimensionless	☑
Vgludem	Vgludem		120.000		☑
Kgludemglu	Kgludemglu		8.000		☑
Kgludemeq	Kgludemeq		10^{10}		☑
Kgludemazglu	Kgludemazglu		0.500		☑
Vglndem	Vglndem		70.000		☑
Kglndemgln	Kglndemgln		2.000		☑
Kglndemeq	Kglndemeq		10^{10}		☑
Kglndemazgln	Kglndemazgln		0.250		☑
Vazglndem	Vazglndem		20.000		☑
Kazglndemazgln	Kazglndemazgln		1.000		☑
Kazglndemeq	Kazglndemeq		10^{10}		☑
Kazglndemazinter	Kazglndemazinter		0.500		☑

Id	Name	SBO	Value	Unit	Constant
Vazgludem	Vazgludem		30.000		☑
Kazgludemazglu	Kazgludemazglu		0.300		☑
Kazgludemeq	Kazgludemeq		10^{10}	dimensionless	☑
Kazgludemazinter	Kazgludemazinter		0.500	dimensionless	☑
Vadp	Vadp		100.000		☑
Kadp	Kadp		0.500		☑
ATPtot	ATPtot		5.370		☑
GStot	GStot		0.014		☑
PIItot	PIItot		0.003		☑
Kd1	Kd1		0.005		☑
Kd2	Kd2		0.150		☑
Kd3	Kd3		0.150		☑
Kd1piiump	Kd1piiump		0.025		☑
Kd2piiump	Kd2piiump		0.150		☑
Kd3piiump	Kd3piiump		0.150		☑
vAPP_GS	maxRateGS		0.000		☐
nAMP	AdenylationStateGS		0.000		☐
PIIKG1	PIIKG1		0.000		☐
PIIUMP3KG3	PIIUMP3KG3		0.000		☐

6 Rules

This is an overview of four rules.

6.1 Rule vAPP_GS

Rule vAPP_GS is an assignment rule for parameter vAPP_GS:

$$\text{vAPP\_GS} = \frac{\text{aamp} \cdot \text{camp}}{\left(1 + 12^{\text{n1amp}} \cdot \left(\frac{[\text{AMP}]}{\text{bamp} \cdot \text{GStot}}\right)^{\text{n1amp}}\right) \cdot \left(1 + 12^{\text{n2amp}} \cdot \left(\frac{[\text{AMP}]}{\text{damp} \cdot \text{GStot}}\right)^{\text{n2amp}}\right)} \cdot \text{Vgs} \quad (1)$$

6.2 Rule nAMP

Rule nAMP is an assignment rule for parameter nAMP:

$$\text{nAMP} = \frac{12 \cdot [\text{AMP}]}{\text{GStot}} \quad (2)$$

6.3 Rule PIIKG1

Rule PIIKG1 is an assignment rule for parameter PIIKG1:

$$\mathrm{PIIKG1} = \frac{\frac{3\cdot[\mathrm{PII}]\cdot[\mathrm{KG}]}{\mathrm{Kd1}}}{1+\frac{3\cdot[\mathrm{KG}]}{\mathrm{Kd1}}+\frac{3\cdot[\mathrm{KG}]^2}{\mathrm{Kd1}\cdot\mathrm{Kd2}}+\frac{[\mathrm{KG}]^3}{\mathrm{Kd1}\cdot\mathrm{Kd2}\cdot\mathrm{Kd3}}} \tag{3}$$

6.4 Rule PIIUMP3KG3

Rule PIIUMP3KG3 is an assignment rule for parameter PIIUMP3KG3:

$$\mathrm{PIIUMP3KG3} = \frac{\frac{[\mathrm{PIIUMP3}]\cdot[\mathrm{KG}]^3}{\mathrm{Kd1piiump}\cdot\mathrm{Kd2piiump}\cdot\mathrm{Kd3piiump}}}{1+\frac{3\cdot[\mathrm{KG}]}{\mathrm{Kd1piiump}}+\frac{3\cdot[\mathrm{KG}]^2}{\mathrm{Kd1piiump}\cdot\mathrm{Kd2piiump}}+\frac{[\mathrm{KG}]^3}{\mathrm{Kd1piiump}\cdot\mathrm{Kd2piiump}\cdot\mathrm{Kd3piiump}}} \tag{4}$$

7 Reactions

This model contains 16 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	vut1	vut1	$\mathrm{PII} + \mathrm{UTP} \xrightleftharpoons{\mathrm{GLN,\ PIIUMP2,\ PIIUMP3}} \mathrm{PIIUMP} + \mathrm{PPi}$	
2	vur1	vur1	$\mathrm{PIIUMP} \xrightleftharpoons{\mathrm{GLN,\ PIIUMP2,\ PIIUMP3}} \mathrm{PII} + \mathrm{UMP}$	
3	vut2	vut2	$\mathrm{PIIUMP} + \mathrm{UTP} \xrightleftharpoons{\mathrm{GLN,\ PII,\ PIIUMP3}} \mathrm{PIIUMP2} + \mathrm{PPi}$	
4	vur2	vur2	$\mathrm{PIIUMP2} \xrightleftharpoons{\mathrm{GLN,\ PIIUMP3}} \mathrm{PIIUMP} + \mathrm{UMP}$	
5	vut3	vut3	$\mathrm{PIIUMP2} + \mathrm{UTP} \xrightleftharpoons{\mathrm{GLN,\ PII,\ PIIUMP}} \mathrm{PIIUMP3} + \mathrm{PPi}$	
6	vur3	vur3	$\mathrm{PIIUMP3} \xrightleftharpoons{\mathrm{GLN,\ PIIUMP}} \mathrm{PIIUMP2} + \mathrm{UMP}$	
7	vad	vad	$\mathrm{GS} \xrightleftharpoons{\mathrm{GLN,\ PII,\ KG}} \mathrm{AMP}$	
8	vdead	vdead	$\mathrm{AMP} \xrightleftharpoons{\mathrm{GLN,\ PII,\ PIIUMP3,\ KG}} \mathrm{GS}$	
9	vgdh	vgdh	$\mathrm{NH4} + \mathrm{KG} + \mathrm{NADPH} \rightleftharpoons \mathrm{GLU} + \mathrm{NADP}$	
10	vgog	vgog	$\mathrm{GLN} + \mathrm{NADPH} + \mathrm{KG} \xrightleftharpoons{\mathrm{AZGLU}} 2\,\mathrm{GLU} + \mathrm{NADP}$	
11	vgs	vgs	$\mathrm{GLU} + \mathrm{ATP} + \mathrm{NH4} \xrightleftharpoons{\mathrm{AMP}} \mathrm{P\_i} + \mathrm{GLN} + \mathrm{ADP}$	
12	vgludem	vgludem	$\mathrm{GLU} \rightleftharpoons \mathrm{AZGLU}$	
13	vazgludem	vazgludem	$\mathrm{AZGLU} \rightleftharpoons \mathrm{AZglu}$	
14	vglndem	vglndem	$\mathrm{GLN} \rightleftharpoons \mathrm{AZGLN}$	
15	vazglndem	vazglndem	$\mathrm{AZGLN} \rightleftharpoons \mathrm{AZgln}$	

№	Id	Name	Reaction Equation	SBO
16	vatpase	vatpase	ADP $\rightleftharpoons$ ATP	

7.1 Reaction vut1

This is a reversible reaction of two reactants forming two products influenced by three modifiers.

Name vut1

Reaction equation

$$\mathrm{PII} + \mathrm{UTP} \xrightleftharpoons{\text{GLN, PIIUMP2, PIIUMP3}} \mathrm{PIIUMP} + \mathrm{PPi} \tag{5}$$

Reactants

Table 6: Properties of each reactant.

Id	Name	SBO
PII	PII	
UTP	UTP	

Modifiers

Table 7: Properties of each modifier.

Id	Name	SBO
GLN	GLN	
PIIUMP2	PIIUMP2	
PIIUMP3	PIIUMP3	

Products

Table 8: Properties of each product.

Id	Name	SBO
PIIUMP	PIIUMP	
PPi	PPi	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \frac{\mathrm{kcatut} \cdot \mathrm{UT} \cdot [\mathrm{UTP}] \cdot [\mathrm{PII}]}{\mathrm{Kutipii} \cdot \mathrm{Kututp} \cdot \left(1 + \frac{[\mathrm{GLN}]}{\mathrm{Kglnut}}\right) \cdot \left(1 + \frac{[\mathrm{UTP}]}{\mathrm{Kututp}} + \frac{[\mathrm{PII}]+[\mathrm{PIIUMP}]+[\mathrm{PIIUMP2}]}{\mathrm{Kutipii}} + \frac{[\mathrm{UTP}]\cdot([\mathrm{PII}]+[\mathrm{PIIUMP}]+[\mathrm{PIIUMP2}])}{\mathrm{Kutipii}\cdot\mathrm{Kututp}} + \frac{[\mathrm{PPi}]\cdot[\mathrm{UTP}]\cdot}{\mathrm{K}}\right.} \tag{6}$$

7.2 Reaction vur1

This is a reversible reaction of one reactant forming two products influenced by three modifiers.

Name vur1

Reaction equation

$$\mathrm{PIIUMP} \xrightleftharpoons{\text{GLN, PIIUMP2, PIIUMP3}} \mathrm{PII} + \mathrm{UMP} \tag{7}$$

Reactant

Table 9: Properties of each reactant.

Id	Name	SBO
PIIUMP	PIIUMP	

Modifiers

Table 10: Properties of each modifier.

Id	Name	SBO
GLN	GLN	
PIIUMP2	PIIUMP2	
PIIUMP3	PIIUMP3	

Products

Table 11: Properties of each product.

Id	Name	SBO
PII	PII	
UMP	UMP	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \frac{\mathrm{kcatur} \cdot \mathrm{UR} \cdot [\mathrm{PIIUMP}]}{\mathrm{Kurpiiump} \cdot \left(1 + \frac{\mathrm{Kglnur}}{[\mathrm{GLN}]}\right) \cdot \left(1 + \frac{\left(1 + \frac{[\mathrm{UMP}]}{\mathrm{Kurump}}\right) \cdot ([\mathrm{PIIUMP}] + [\mathrm{PIIUMP2}] + [\mathrm{PIIUMP3}])}{\mathrm{Kurpiiump}}\right)} \tag{8}$$

7.3 Reaction `vut2`

This is a reversible reaction of two reactants forming two products influenced by three modifiers.

Name vut2

Reaction equation

$$\mathrm{PIIUMP} + \mathrm{UTP} \underset{}{\overset{\mathrm{GLN,\ PII,\ PIIUMP3}}{\rightleftharpoons}} \mathrm{PIIUMP2} + \mathrm{PPi} \tag{9}$$

Reactants

Table 12: Properties of each reactant.

Id	Name	SBO
`PIIUMP`	PIIUMP	
`UTP`	UTP	

Modifiers

Table 13: Properties of each modifier.

Id	Name	SBO
`GLN`	GLN	
`PII`	PII	
`PIIUMP3`	PIIUMP3	

Products

Table 14: Properties of each product.

Id	Name	SBO
`PIIUMP2`	PIIUMP2	
`PPi`	PPi	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \frac{\mathrm{kcatut} \cdot \mathrm{UT} \cdot [\mathrm{UTP}] \cdot [\mathrm{PIIUMP}]}{\mathrm{Kutipii} \cdot \mathrm{Kututp} \cdot \left(1 + \frac{[\mathrm{GLN}]}{\mathrm{Kglnut}}\right) \cdot \left(1 + \frac{[\mathrm{UTP}]}{\mathrm{Kututp}} + \frac{[\mathrm{PII}]+[\mathrm{PIIUMP}]+[\mathrm{PIIUMP2}]}{\mathrm{Kutipii}} + \frac{[\mathrm{UTP}]\cdot([\mathrm{PII}]+[\mathrm{PIIUMP}]+[\mathrm{PIIUMP2}])}{\mathrm{Kutipii}\cdot\mathrm{Kututp}} + \frac{[\mathrm{PPi}]\cdot[\mathrm{UTP}]}{\mathrm{K}}\right.} \tag{10}$$

7.4 Reaction `vur2`

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

Name vur2

Reaction equation

$$\mathrm{PIIUMP2} \xrightleftharpoons{\mathrm{GLN},\ \mathrm{PIIUMP3}} \mathrm{PIIUMP} + \mathrm{UMP} \tag{11}$$

Reactant

Table 15: Properties of each reactant.

Id	Name	SBO
`PIIUMP2`	PIIUMP2	

Modifiers

Table 16: Properties of each modifier.

Id	Name	SBO
`GLN`	GLN	
`PIIUMP3`	PIIUMP3	

Products

Table 17: Properties of each product.

Id	Name	SBO
`PIIUMP`	PIIUMP	
`UMP`	UMP	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \frac{\mathrm{kcatur} \cdot \mathrm{UR} \cdot [\mathrm{PIIUMP2}]}{\mathrm{Kurpiiump} \cdot \left(1 + \frac{\mathrm{Kglnur}}{[\mathrm{GLN}]}\right) \cdot \left(1 + \frac{\left(1 + \frac{[\mathrm{UMP}]}{\mathrm{Kurump}}\right) \cdot ([\mathrm{PIIUMP}] + [\mathrm{PIIUMP2}] + [\mathrm{PIIUMP3}])}{\mathrm{Kurpiiump}}\right)} \tag{12}$$

7.5 Reaction `vut3`

This is a reversible reaction of two reactants forming two products influenced by three modifiers.

Name vut3

Reaction equation

$$\mathrm{PIIUMP2} + \mathrm{UTP} \overset{\mathrm{GLN,\ PII,\ PIIUMP}}{\rightleftharpoons} \mathrm{PIIUMP3} + \mathrm{PPi} \tag{13}$$

Reactants

Table 18: Properties of each reactant.

Id	Name	SBO
`PIIUMP2`	PIIUMP2	
`UTP`	UTP	

Modifiers

Table 19: Properties of each modifier.

Id	Name	SBO
`GLN`	GLN	
`PII`	PII	
`PIIUMP`	PIIUMP	

Products

Table 20: Properties of each product.

Id	Name	SBO
PIIUMP3	PIIUMP3	
PPi	PPi	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \frac{\mathrm{kcatut} \cdot \mathrm{UT} \cdot [\mathrm{UTP}] \cdot [\mathrm{PIIUMP2}]}{\mathrm{Kutipii} \cdot \mathrm{Kututp} \cdot \left(1 + \frac{[\mathrm{GLN}]}{\mathrm{Kglnut}}\right) \cdot \left(1 + \frac{[\mathrm{UTP}]}{\mathrm{Kututp}} + \frac{[\mathrm{PII}]+[\mathrm{PIIUMP}]+[\mathrm{PIIUMP2}]}{\mathrm{Kutipii}} + \frac{[\mathrm{UTP}]\cdot([\mathrm{PII}]+[\mathrm{PIIUMP}]+[\mathrm{PIIUMP2}])}{\mathrm{Kutipii}\cdot\mathrm{Kututp}} + \frac{[\mathrm{PPi}]\cdot[\mathrm{UTP}]}{\mathrm{K}}\right.} \quad (14)$$

7.6 Reaction vur3

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

Name vur3

Reaction equation

$$\mathrm{PIIUMP3} \overset{\mathrm{GLN,\ PIIUMP}}{\rightleftharpoons} \mathrm{PIIUMP2} + \mathrm{UMP} \quad (15)$$

Reactant

Table 21: Properties of each reactant.

Id	Name	SBO
PIIUMP3	PIIUMP3	

Modifiers

Table 22: Properties of each modifier.

Id	Name	SBO
GLN	GLN	
PIIUMP	PIIUMP	

Products

Table 23: Properties of each product.

Id	Name	SBO
PIIUMP2	PIIUMP2	
UMP	UMP	

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \frac{\mathrm{kcatur} \cdot \mathrm{UR} \cdot [\mathrm{PIIUMP3}]}{\mathrm{Kurpiiump} \cdot \left(1 + \frac{\mathrm{Kglnur}}{[\mathrm{GLN}]}\right) \cdot \left(1 + \frac{\left(1 + \frac{[\mathrm{UMP}]}{\mathrm{Kurump}}\right) \cdot ([\mathrm{PIIUMP}] + [\mathrm{PIIUMP2}] + [\mathrm{PIIUMP3}])}{\mathrm{Kurpiiump}}\right)} \tag{16}$$

7.7 Reaction vad

This is a reversible reaction of one reactant forming one product influenced by three modifiers.

Name vad

Reaction equation

$$\mathrm{GS} \overset{\mathrm{GLN,\ PII,\ KG}}{\rightleftharpoons} \mathrm{AMP} \tag{17}$$

Reactant

Table 24: Properties of each reactant.

Id	Name	SBO
GS	GS	

Modifiers

Table 25: Properties of each modifier.

Id	Name	SBO
GLN	GLN	
PII	PII	
KG	KG	

Product

Table 26: Properties of each product.

Id	Name	SBO
AMP	AMP	

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \mathrm{vol}\,(\mathrm{compartment}) \tag{18}$$
$$\cdot \frac{\mathrm{Vad}\cdot[\mathrm{GS}]\cdot\left(\frac{\mathrm{b1}\cdot[\mathrm{GLN}]}{\mathrm{Kadgln}}+\frac{3\cdot\mathrm{a1}\cdot[\mathrm{KG}]\cdot[\mathrm{PII}]}{\mathrm{Kadpiikg}\cdot\mathrm{Kd1}\cdot\left(1+\frac{3\cdot[\mathrm{KG}]}{\mathrm{Kd1}}+\frac{3\cdot[\mathrm{KG}]^2}{\mathrm{Kd1}\cdot\mathrm{Kd2}}+\frac{[\mathrm{KG}]^3}{\mathrm{Kd1}\cdot\mathrm{Kd2}\cdot\mathrm{Kd3}}\right)}+\frac{3\cdot\mathrm{c1}\cdot[\mathrm{KG}]\cdot[\mathrm{GLN}]\cdot[\mathrm{PII}]}{\mathrm{Kadgln}\cdot\mathrm{Kadpiikg}\cdot\mathrm{Kd1}\cdot\left(1+\frac{3\cdot[\mathrm{KG}]}{\mathrm{Kd1}}+\frac{3\cdot[\mathrm{KG}]^2}{\mathrm{Kd1}\cdot\mathrm{Kd2}}+\frac{[\mathrm{KG}]^3}{\mathrm{Kd1}\cdot\mathrm{Kd2}\cdot\mathrm{Kd3}}\right.}\right)}{(\mathrm{Kadgs}+[\mathrm{GS}])\cdot\left(1+\frac{[\mathrm{GLN}]}{\mathrm{Kadgln}}+\frac{3\cdot[\mathrm{KG}]\cdot[\mathrm{PII}]}{\mathrm{Kadpiikg}\cdot\mathrm{Kd1}\cdot\left(1+\frac{3\cdot[\mathrm{KG}]}{\mathrm{Kd1}}+\frac{3\cdot[\mathrm{KG}]^2}{\mathrm{Kd1}\cdot\mathrm{Kd2}}+\frac{[\mathrm{KG}]^3}{\mathrm{Kd1}\cdot\mathrm{Kd2}\cdot\mathrm{Kd3}}\right)}+\frac{3\cdot[\mathrm{KG}]\cdot[\mathrm{GLN}]\cdot[\mathrm{PII}]}{\mathrm{d1}\cdot\mathrm{Kadgln}\cdot\mathrm{Kadpiikg}\cdot\mathrm{Kd1}\cdot\left(1+\frac{3\cdot[\mathrm{KG}]}{\mathrm{Kd1}}+\frac{3\cdot[\mathrm{KG}]^2}{\mathrm{Kd1}\cdot\mathrm{Kd2}}+\frac{[\mathrm{KG}]^3}{\mathrm{Kd1}\cdot\mathrm{Kd2}\cdot\mathrm{Kd3}}\right.}\right)}$$

7.8 Reaction vdead

This is a reversible reaction of one reactant forming one product influenced by four modifiers.

Name vdead

Reaction equation

$$\mathrm{AMP} \xrightleftharpoons{\mathrm{GLN,\ PII,\ PIIUMP3,\ KG}} \mathrm{GS} \tag{19}$$

Reactant

Table 27: Properties of each reactant.

Id	Name	SBO
AMP	AMP	

Modifiers

Table 28: Properties of each modifier.

Id	Name	SBO
GLN	GLN	
PII	PII	

Id	Name	SBO
PIIUMP3	PIIUMP3	
KG	KG	

Product

Table 29: Properties of each product.

Id	Name	SBO
GS	GS	

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \frac{\mathrm{Vdead} \cdot [\mathrm{AMP}] \cdot \left(\frac{\mathrm{f1} \cdot [\mathrm{GLN}]}{\mathrm{Kdeadgln}} + \frac{3 \cdot \mathrm{e1} \cdot [\mathrm{KG}] \cdot [\mathrm{PII}]}{\mathrm{Kd1} \cdot \mathrm{Kdeadpiikg} \cdot \left(1 + \frac{3 \cdot [\mathrm{KG}]}{\mathrm{Kd1}} + \frac{3 \cdot [\mathrm{KG}]^2}{\mathrm{Kd1} \cdot \mathrm{Kd2}} + \frac{[\mathrm{KG}]^3}{\mathrm{Kd1} \cdot \mathrm{Kd2} \cdot \mathrm{Kd3}}\right)} + \frac{3 \cdot \mathrm{h1} \cdot [\mathrm{KG}] \cdot [\mathrm{GLN}] \cdot [\mathrm{PI}}{\mathrm{Kd1} \cdot \mathrm{Kdeadgln} \cdot \mathrm{Kdeadpiikg} \cdot \left(1 + \frac{3 \cdot [\mathrm{KG}]}{\mathrm{Kd1}} + \right.} \right)}{(\mathrm{Kdeadgsa} + [\mathrm{AMP}]) \cdot \left(1 + \frac{[\mathrm{GLN}]}{\mathrm{Kdeadgln}} + \frac{3 \cdot [\mathrm{KG}] \cdot [\mathrm{PII}]}{\mathrm{Kd1} \cdot \mathrm{Kdeadpiikg} \cdot \left(1 + \frac{3 \cdot [\mathrm{KG}]}{\mathrm{Kd1}} + \frac{3 \cdot [\mathrm{KG}]^2}{\mathrm{Kd1} \cdot \mathrm{Kd2}} + \frac{[\mathrm{KG}]^3}{\mathrm{Kd1} \cdot \mathrm{Kd2} \cdot \mathrm{Kd3}}\right)} + \frac{3 \cdot [\mathrm{KG}] \cdot [\mathrm{GLN}] \cdot [\mathrm{P}}{\mathrm{Kd1} \cdot \mathrm{Kdeadgln} \cdot \mathrm{Kdeadpiikg} \cdot \left(1 + \frac{3 \cdot [\mathrm{KG}]}{\mathrm{Kd1}} + \right.} \right)} \quad (20)$$

7.9 Reaction vgdh

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

Name vgdh

Reaction equation

$$\mathrm{NH4} + \mathrm{KG} + \mathrm{NADPH} \rightleftharpoons \mathrm{GLU} + \mathrm{NADP} \quad (21)$$

Reactants

Table 30: Properties of each reactant.

Id	Name	SBO
NH4	NH4	
KG	KG	
NADPH	NADPH	

Products

Table 31: Properties of each product.

Id	Name	SBO
GLU	GLU	
NADP	NADP	

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \frac{\mathrm{Vgdh} \cdot \left([\mathrm{KG}] \cdot [\mathrm{NADPH}] \cdot [\mathrm{NH4}] - \frac{[\mathrm{NADP}] \cdot [\mathrm{GLU}]}{\mathrm{Keqgdh}}\right)}{\mathrm{Kgdhkg} \cdot \mathrm{Kgdhnadph} \cdot \mathrm{Kgdhnh} \cdot \left(1 + \frac{[\mathrm{NADP}]}{\mathrm{Kgdhnadp}} + \frac{[\mathrm{NADPH}]}{\mathrm{Kgdhnadph}}\right) \cdot \left(1 + \frac{[\mathrm{NH4}]}{\mathrm{Kgdhnh}}\right) \cdot \left(1 + \frac{[\mathrm{KG}]}{\mathrm{Kgdhkg}} + \frac{[\mathrm{GLU}]}{\mathrm{Kgdhglu}}\right)} \tag{22}$$

7.10 Reaction vgog

This is a reversible reaction of three reactants forming two products influenced by one modifier.

Name vgog

Reaction equation

$$\mathrm{GLN} + \mathrm{NADPH} + \mathrm{KG} \xrightleftharpoons{\mathrm{AZGLU}} 2\,\mathrm{GLU} + \mathrm{NADP} \tag{23}$$

Reactants

Table 32: Properties of each reactant.

Id	Name	SBO
GLN	GLN	
NADPH	NADPH	
KG	KG	

Modifier

Table 33: Properties of each modifier.

Id	Name	SBO
AZGLU	AZGLU	

Id	Name	SBO

Products

Table 34: Properties of each product.

Id	Name	SBO
GLU	GLU	
NADP	NADP	

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = \mathrm{vol}\,(\mathrm{compartment}) \cdot \frac{[\mathrm{KG}] \cdot [\mathrm{NADPH}] \cdot \mathrm{Vgog} \cdot [\mathrm{GLN}]}{\mathrm{Kgoggln} \cdot \mathrm{Kgogkg} \cdot \mathrm{Kgognadph} \cdot \left(1 + \frac{[\mathrm{NADP}]}{\mathrm{Kgognadp}} + \frac{[\mathrm{NADPH}]}{\mathrm{Kgognadph}}\right) \cdot \left(1 + \frac{[\mathrm{AZGLU}]}{\mathrm{Kgogaz}}\right) \cdot \left(1 + \frac{[\mathrm{KG}]}{\mathrm{Kgogkg}} + \frac{[\mathrm{GLU}]}{\mathrm{Kgogglu}}\right) \cdot \left(1 + \text{I}\right.} \tag{24}$$

7.11 Reaction vgs

This is a reversible reaction of three reactants forming three products influenced by one modifier.

Name vgs

Reaction equation

$$\mathrm{GLU} + \mathrm{ATP} + \mathrm{NH4} \overset{\mathrm{AMP}}{\rightleftharpoons} \mathrm{P\_i} + \mathrm{GLN} + \mathrm{ADP} \tag{25}$$

Reactants

Table 35: Properties of each reactant.

Id	Name	SBO
GLU	GLU	
ATP	ATP	
NH4	NH4	

Modifier

Table 36: Properties of each modifier.

Id	Name	SBO
AMP	AMP	

Products

Table 37: Properties of each product.

Id	Name	SBO
P_i	P_i	
GLN	GLN	
ADP	ADP	

Kinetic Law

Derived unit contains undeclared units

$$v_{11} = \mathrm{vol}\,(\mathrm{compartment}) \cdot \frac{\mathrm{aamp} \cdot \mathrm{camp} \cdot \mathrm{Vgs} \cdot \left(\left(\frac{[\mathrm{P\_i}] \cdot [\mathrm{ADP}] \cdot [\mathrm{GLN}]}{\mathrm{Keq}}\right) + [}{\mathrm{Kgsatp} \cdot \mathrm{Kgsglu} \cdot \mathrm{Kgsnh} \cdot \left(1 + \frac{[\mathrm{P\_i}]}{\mathrm{Kgspi}} + \frac{[\mathrm{ADP}]}{\mathrm{Kgsadp}} + \frac{[\mathrm{P\_i}] \cdot [\mathrm{ADP}]}{\mathrm{Kgsadp} \cdot \mathrm{Kgspi}} + \frac{[\mathrm{ATP}]}{\mathrm{Kgsatp}}\right) \cdot \left(1 + \frac{[\mathrm{NH4}]}{\mathrm{Kgsnh}} + \frac{[\mathrm{GLN}]}{\mathrm{Kgsgln}} + \frac{[\mathrm{NH4}] \cdot [\mathrm{GLN}]}{\mathrm{Kgsgln} \cdot \mathrm{Kgsnh}} + \frac{[\mathrm{GL}}{\mathrm{Kgs}}\right.} \tag{26}$$

7.12 Reaction vgludem

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

Name vgludem

Reaction equation

$$\mathrm{GLU} \rightleftharpoons \mathrm{AZGLU} \tag{27}$$

Reactant

Table 38: Properties of each reactant.

Id	Name	SBO
GLU	GLU	

Product

Table 39: Properties of each product.

Id	Name	SBO
AZGLU	AZGLU	

Kinetic Law

Derived unit contains undeclared units

$$v_{12} = \mathrm{vol}\,(\mathrm{compartment}) \cdot \frac{\mathrm{Vgludem} \cdot \left(\left(\frac{[\mathrm{AZGLU}]}{\mathrm{Kgludemeq}}\right) + [\mathrm{GLU}]\right)}{\mathrm{Kgludemglu} \cdot \left(1 + \frac{[\mathrm{AZGLU}]}{\mathrm{Kgludemazglu}} + \frac{[\mathrm{GLU}]}{\mathrm{Kgludemglu}}\right)} \tag{28}$$

7.13 Reaction vazgludem

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

Name vazgludem

Reaction equation

$$\mathrm{AZGLU} \rightleftharpoons \mathrm{AZglu} \tag{29}$$

Reactant

Table 40: Properties of each reactant.

Id	Name	SBO
AZGLU	AZGLU	

Product

Table 41: Properties of each product.

Id	Name	SBO
AZglu	AZglu	

Kinetic Law

Derived unit contains undeclared units

$$v_{13} = \mathrm{vol}\left(\mathrm{compartment}\right) \cdot \frac{\mathrm{Vazgludem} \cdot \left(\left(\frac{[\mathrm{AZglu}]}{\mathrm{Kazgludemeq}}\right) + [\mathrm{AZGLU}]\right)}{\mathrm{Kazgludemazglu} \cdot \left(1 + \frac{[\mathrm{AZglu}]}{\mathrm{Kazgludemazinter}} + \frac{[\mathrm{AZGLU}]}{\mathrm{Kazgludemazglu}}\right)} \tag{30}$$

7.14 Reaction `vglndem`

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

Name vglndem

Reaction equation

$$\mathrm{GLN} \rightleftharpoons \mathrm{AZGLN} \tag{31}$$

Reactant

Table 42: Properties of each reactant.

Id	Name	SBO
`GLN`	GLN	

Product

Table 43: Properties of each product.

Id	Name	SBO
`AZGLN`	AZGLN	

Kinetic Law

Derived unit contains undeclared units

$$v_{14} = \mathrm{vol}\left(\mathrm{compartment}\right) \cdot \frac{\mathrm{Vglndem} \cdot \left(\left(\frac{[\mathrm{AZGLN}]}{\mathrm{Kglndemeq}}\right) + [\mathrm{GLN}]\right)}{\mathrm{Kglndemgln} \cdot \left(1 + \frac{[\mathrm{AZGLN}]}{\mathrm{Kglndemazgln}} + \frac{[\mathrm{GLN}]}{\mathrm{Kglndemgln}}\right)} \tag{32}$$

7.15 Reaction `vazglndem`

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

Name vazglndem

Reaction equation

$$\mathrm{AZGLN} \rightleftharpoons \mathrm{AZgln} \tag{33}$$

Reactant

Table 44: Properties of each reactant.

Id	Name	SBO
AZGLN	AZGLN	

Product

Table 45: Properties of each product.

Id	Name	SBO
AZgln	AZgln	

Kinetic Law

Derived unit contains undeclared units

$$v_{15} = \mathrm{vol}\left(\mathrm{compartment}\right) \cdot \frac{\mathrm{Vazglndem} \cdot \left(\left(\frac{[\mathrm{AZgln}]}{\mathrm{Kazglndemeq}}\right) + [\mathrm{AZGLN}]\right)}{\mathrm{Kazglndemazgln} \cdot \left(1 + \frac{[\mathrm{AZgln}]}{\mathrm{Kazglndemazinter}} + \frac{[\mathrm{AZGLN}]}{\mathrm{Kazglndemazgln}}\right)} \tag{34}$$

7.16 Reaction vatpase

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

Name vatpase

Reaction equation

$$\mathrm{ADP} \rightleftharpoons \mathrm{ATP} \tag{35}$$

Reactant

Table 46: Properties of each reactant.

Id	Name	SBO
ADP	ADP	

Product

Table 47: Properties of each product.

Id	Name	SBO
ATP	ATP	

Kinetic Law

Derived unit contains undeclared units

$$v_{16} = \mathrm{vol}\,(\mathrm{compartment}) \cdot \frac{\mathrm{Vadp} \cdot [\mathrm{ADP}]}{\mathrm{Kadp} + [\mathrm{ADP}]} \tag{36}$$

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.

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.

8.1 Species PII

Name PII

Initial concentration $0.0030\ \mathrm{mol} \cdot \mathrm{l}^{-1}$

This species takes part in six reactions (as a reactant in vut1 and as a product in vur1 and as a modifier in vut2, vut3, vad, vdead).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{PII} = v_2 - v_1 \tag{37}$$

8.2 Species UTP

Name UTP

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

This species takes part in three reactions (as a reactant in vut1, vut2, vut3), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{UTP} = 0 \tag{38}$$

8.3 Species PIIUMP

Name PIIUMP

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

This species takes part in six reactions (as a reactant in vur1, vut2 and as a product in vut1, vur2 and as a modifier in vut3, vur3).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{PIIUMP} = v_1 + v_4 - v_2 - v_3 \tag{39}$$

8.4 Species PPi

Name PPi

Initial concentration $0.05\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in three reactions (as a product in vut1, vut2, vut3), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{PPi} = 0 \tag{40}$$

8.5 Species GLN

Name GLN

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

This species takes part in eleven reactions (as a reactant in vgog, vglndem and as a product in vgs and as a modifier in vut1, vur1, vut2, vur2, vut3, vur3, vad, vdead).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{GLN} = v_{11} - v_{10} - v_{14} \tag{41}$$

8.6 Species PIIUMP2

Name PIIUMP2

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

This species takes part in six reactions (as a reactant in vur2, vut3 and as a product in vut2, vur3 and as a modifier in vut1, vur1).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{PIIUMP2} = v_3 + v_6 - v_4 - v_5 \tag{42}$$

8.7 Species PIIUMP3

Name PIIUMP3

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

This species takes part in seven reactions (as a reactant in vur3 and as a product in vut3 and as a modifier in vut1, vur1, vut2, vur2, vdead).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{PIIUMP3} = v_5 - v_6 \tag{43}$$

8.8 Species UMP

Name UMP

Initial concentration $0.01\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in three reactions (as a product in vur1, vur2, vur3), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{UMP} = 0 \tag{44}$$

8.9 Species GS

Name GS

Initial concentration $0.014\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in vad and as a product in vdead).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{GS} = v_8 - v_7 \tag{45}$$

8.10 Species AMP

Name AMP

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

This species takes part in three reactions (as a reactant in vdead and as a product in vad and as a modifier in vgs).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{AMP} = v_7 - v_8 \tag{46}$$

8.11 Species NH4

Name NH4

Initial concentration $0.05\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{NH4} = 0 \tag{47}$$

8.12 Species KG

Name KG

Initial concentration $0.2\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in four reactions (as a reactant in vgdh, vgog and as a modifier in vad, vdead), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{KG} = 0 \tag{48}$$

8.13 Species NADPH

Name NADPH

Initial concentration $0.15\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{NADPH} = 0 \tag{49}$$

8.14 Species GLU

Name GLU

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

This species takes part in four reactions (as a reactant in vgs, vgludem and as a product in vgdh, vgog).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{GLU} = v_9 + 2\,v_{10} - v_{11} - v_{12} \tag{50}$$

8.15 Species NADP

Name NADP

Initial concentration $0.05\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{NADP} = 0 \tag{51}$$

8.16 Species AZGLU

Name AZGLU

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

This species takes part in three reactions (as a reactant in vazgludem and as a product in vgludem and as a modifier in vgog).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{AZGLU} = v_{12} - v_{13} \tag{52}$$

8.17 Species ATP

Name ATP

Initial concentration $2.685\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in vgs and as a product in vatpase).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ATP} = v_{16} - v_{11} \tag{53}$$

8.18 Species ADP

Name ADP

Initial concentration $2.685\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in vatpase and as a product in vgs).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ADP} = v_{11} - v_{16} \tag{54}$$

8.19 Species AZglu

Name AZglu

Initial concentration $0.1\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{AZglu} = 0 \tag{55}$$

8.20 Species AZGLN

Name AZGLN

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

This species takes part in two reactions (as a reactant in vazglndem and as a product in vglndem).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{AZGLN} = v_{14} - v_{15} \tag{56}$$

8.21 Species AZgln

Name AZgln

Initial concentration $0.1\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{AZgln} = 0 \tag{57}$$

8.22 Species P_i

Name P_i

Initial concentration $10\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{P\_i} = 0 \tag{58}$$

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