SBML Model Report

Model name: "Thiaville2016 - Folate pathway model (PanB overexpression and THF regulation)"

May 17, 2018

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by the following two authors: Christopher Henry[1] and Matthew Grant Roberts[2] at March third 2015 at 0:36 a. m. and last time modified at March twelveth 2018 at 3:50 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	1
species types	0	species	17
events	0	constraints	0
reactions	10	function definitions	3
global parameters	0	unit definitions	2
rules	0	initial assignments	0

Model Notes

Henry2016 Folate pathway model with inducedPanB reaction

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This model is described in the article:Experimental and Metabolic Modeling Evidence for a Folate-Cleaving Side-Activity of Ketopantoate Hydroxymethyltransferase (PanB).Thiaville JJ, Frelin O, Garca-Salinas C, Harrison K, Hasnain G, Horenstein NA, Daz de la Garza RI, Henry CS, Hanson AD, de Crcy-Lagard V.Front Microbiol 2016; 7: 431

Abstract:

Tetrahydrofolate (THF) and its one-carbon derivatives, collectively termed folates, are essential cofactors, but are inherently unstable. While it is clear that chemical oxidation can cleave folates or damage their pterin precursors, very little is known about enzymatic damage to these molecules or about whether the folate biosynthesis pathway responds adaptively to damage to its end-products. The presence of a duplication of the gene encoding the folate biosynthesis enzyme 6-hydroxymethyl-7,8-dihydropterin pyrophosphokinase (FolK) in many sequenced bacterial genomes combined with a strong chromosomal clustering of the folK gene with panB, encoding the 5,10-methylene-THF-dependent enzyme ketopantoate hydroxymethyltransferase, led us to infer that PanB has a side activity that cleaves 5,10-methylene-THF, yielding a pterin product that is recycled by FolK. Genetic and metabolic analyses of Escherichia coli strains showed that overexpression of PanB leads to accumulation of the likely folate cleavage product 6-hydroxymethylpterin and other pterins in cells and medium, and-unexpectedly-to a 46% increase in total folate content. In silico modeling of the folate biosynthesis pathway showed that these observations are consistent with the in vivo cleavage of 5,10-methylene-THF by a side-activity of PanB, with FolK-mediated recycling of the pterin cleavage product, and with regulation of folate biosynthesis by folates or their damage products.

2 Unit Definitions

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

2.1 Unit `volume`

Name volume

Definition ml

2.2 Unit `substance`

Name substance

Definition mmol

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 ml.

Name compartment

4 Species

This model contains 17 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 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
H2_HMPt	H2-HMPt	compartment	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	☐	☐
ATP	ATP	compartment	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	☑	☑
H2_HMPterinPP	H2-HMPterinPP	compartment	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	☐	☐
AMP	AMP	compartment	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	☑	☑
p_ABA	p-ABA	compartment	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	☐	☐
PPi	PPi	compartment	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	☑	☑
H2_Pteroate	H2-Pteroate	compartment	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	☐	☐
L_Glutamate	L-Glutamate	compartment	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	☑	☑
Phosphate	Phosphate	compartment	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	☑	☑
ADP	ADP	compartment	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	☑	☑
DHF	DHF	compartment	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	☐	☐
L_serine	L-serine	compartment	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	☑	☑
Glycine	Glycine	compartment	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	☑	☑
NADP	NADP	compartment	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	☑	☑
NADPH	NADPH	compartment	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	☑	☑
THF	THF	compartment	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	☐	☐
CH2_THF	CH2-THF	compartment	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	☐	☐

5 Function definitions

This is an overview of three function definitions.

5.1 Function definition Constant_flux__irreversible

Name Constant flux (irreversible)

Argument v

Mathematical Expression

$$\mathrm{v} \tag{1}$$

5.2 Function definition Henri_Michaelis_Menten__irreversible__1

Name Henri-Michaelis-Menten (irreversible)_1

Arguments Km, [THF], V

Mathematical Expression

$$\frac{\mathrm{V} \cdot [\mathrm{THF}]}{\mathrm{Km} + [\mathrm{THF}]} \tag{2}$$

5.3 Function definition Henri_Michaelis_Menten__irreversible__2

Name Henri-Michaelis-Menten (irreversible)_2

Arguments [CH2_THF], Km, V

Mathematical Expression

$$\frac{\mathrm{V} \cdot [\mathrm{CH2\_THF}]}{\mathrm{Km} + [\mathrm{CH2\_THF}]} \tag{3}$$

6 Reactions

This model contains ten 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 4: Overview of all reactions

№	Id	Name	Reaction Equation	SBO
1	FolK	FolK	$ATP + H2\_HMPt \longrightarrow AMP + H2\_HMPterinPP$	
2	FolP	FolP	$p\_ABA + H2\_HMPterinPP \longrightarrow PPi + H2\_Pteroate$	
3	FolC	FolC	$L\_Glutamate + ATP + H2\_Pteroate \longrightarrow DHF + ADP + Phosphate$	
4	GlyA	GlyA	$THF + L\_serine \rightleftharpoons CH2\_THF + Glycine$	
5	FolA	FolA	$DHF + NADPH \longrightarrow NADP + THF$	
6	PanB	PanB	$CH2\_THF \longrightarrow H2\_HMPt + p\_ABA$	
7	p_ABA-_production	p-ABA_production	$\emptyset \longrightarrow p\_ABA$	
8	H2_HMPt-_production	H2-HMPt_production	$\emptyset \longrightarrow H2\_HMPt$	
9	THF_drain	THF_drain	$THF \longrightarrow \emptyset$	
10	CH2_THF_drain	CH2-THF_drain	$CH2\_THF \longrightarrow \emptyset$	

6.1 Reaction FolK

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

Name FolK

Reaction equation

$$\mathrm{ATP} + \mathrm{H2\_HMPt} \longrightarrow \mathrm{AMP} + \mathrm{H2\_HMPterinPP} \tag{4}$$

Reactants

Table 5: Properties of each reactant.

Id	Name	SBO
ATP	ATP	
H2_HMPt	H2-HMPt	

Products

Table 6: Properties of each product.

Id	Name	SBO
AMP	AMP	
H2_HMPterinPP	H2-HMPterinPP	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{k1} \cdot [\mathrm{ATP}] \cdot [\mathrm{H2\_HMPt}] \tag{5}$$

Table 7: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		24.8		☑

6.2 Reaction FolP

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

Name FolP

Reaction equation

$$\text{p\_ABA} + \text{H2\_HMPterinPP} \longrightarrow \text{PPi} + \text{H2\_Pteroate} \tag{6}$$

Reactants

Table 8: Properties of each reactant.

Id	Name	SBO
p_ABA	p-ABA	
H2_HMPterinPP	H2-HMPterinPP	

Products

Table 9: Properties of each product.

Id	Name	SBO
PPi	PPi	
H2_Pteroate	H2-Pteroate	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \text{vol}\,(\text{compartment}) \cdot \text{k1} \cdot [\text{p\_ABA}] \cdot [\text{H2\_HMPterinPP}] \tag{7}$$

Table 10: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		8000.0		☑

6.3 Reaction FolC

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

Name FolC

Reaction equation

$$\text{L\_Glutamate} + \text{ATP} + \text{H2\_Pteroate} \longrightarrow \text{DHF} + \text{ADP} + \text{Phosphate} \tag{8}$$

Reactants

Table 11: Properties of each reactant.

Id	Name	SBO
L_Glutamate	L-Glutamate	
ATP	ATP	
H2_Pteroate	H2-Pteroate	

Products

Table 12: Properties of each product.

Id	Name	SBO
DHF	DHF	
ADP	ADP	
Phosphate	Phosphate	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \text{vol}(\text{compartment}) \cdot \text{k1} \cdot [\text{L\_Glutamate}] \cdot [\text{ATP}] \cdot [\text{H2\_Pteroate}] \tag{9}$$

Table 13: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		10029.0		☑

6.4 Reaction GlyA

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

Name GlyA

Reaction equation

$$\mathrm{THF} + \mathrm{L\_serine} \rightleftharpoons \mathrm{CH2\_THF} + \mathrm{Glycine} \tag{10}$$

Reactants

Table 14: Properties of each reactant.

Id	Name	SBO
THF	THF	
L_serine	L-serine	

Products

Table 15: Properties of each product.

Id	Name	SBO
CH2_THF	CH2-THF	
Glycine	Glycine	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \mathrm{vol}\,(\mathrm{compartment}) \cdot (\mathrm{k1} \cdot [\mathrm{THF}] \cdot [\mathrm{L\_serine}] - \mathrm{k2} \cdot [\mathrm{CH2\_THF}] \cdot [\mathrm{Glycine}]) \tag{11}$$

Table 16: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		4080.0		☑
k2	k2		2000.0		☑

6.5 Reaction FolA

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

Name FolA

Reaction equation

$$\mathrm{DHF} + \mathrm{NADPH} \longrightarrow \mathrm{NADP} + \mathrm{THF} \tag{12}$$

Reactants

Table 17: Properties of each reactant.

Id	Name	SBO
DHF	DHF	
NADPH	NADPH	

Products

Table 18: Properties of each product.

Id	Name	SBO
NADP	NADP	
THF	THF	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{k1} \cdot [\mathrm{DHF}] \cdot [\mathrm{NADPH}] \tag{13}$$

Table 19: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		86170.0		☑

6.6 Reaction PanB

This is an irreversible reaction of one reactant forming two products.

Name PanB

Reaction equation

$$\text{CH2\_THF} \longrightarrow \text{H2\_HMPt} + \text{p\_ABA} \tag{14}$$

Reactant

Table 20: Properties of each reactant.

Id	Name	SBO
CH2_THF	CH2-THF	

Products

Table 21: Properties of each product.

Id	Name	SBO
H2_HMPt	H2-HMPt	
p_ABA	p-ABA	

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \text{vol}\,(\text{compartment}) \cdot \text{k1} \cdot [\text{CH2\_THF}] \tag{15}$$

Table 22: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		0.008		☑

6.7 Reaction p_ABA_production

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

Name p-ABA_production

Reaction equation

$$\emptyset \longrightarrow \text{p\_ABA} \tag{16}$$

Product

Table 23: Properties of each product.

Id	Name	SBO
p_ABA	p-ABA	

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \text{vol}\,(\text{compartment}) \cdot \text{Constant\_flux\_\_irreversible}\,(\text{v}) \tag{17}$$

$$\text{Constant\_flux\_\_irreversible}\,(\text{v}) = \text{v} \tag{18}$$

$$\text{Constant\_flux\_\_irreversible}\,(\text{v}) = \text{v} \tag{19}$$

Table 24: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
v	v		$2.35 \cdot 10^{-7}$		☑

6.8 Reaction H2_HMPt_production

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

Name H2-HMPt_production

Reaction equation

$$\emptyset \longrightarrow \text{H2\_HMPt} \tag{20}$$

Product

Table 25: Properties of each product.

Id	Name	SBO
H2_HMPt	H2-HMPt	

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \text{vol}\,(\text{compartment}) \cdot \text{Constant\_flux\_\_irreversible}\,(\text{v}) \tag{21}$$

$$\text{Constant\_flux\_\_irreversible}\,(\text{v}) = \text{v} \tag{22}$$

$$\text{Constant\_flux\_\_irreversible}\,(\text{v}) = \text{v} \tag{23}$$

Table 26: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
v	v		$2.35 \cdot 10^{-7}$		☑

6.9 Reaction THF_drain

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

Name THF_drain

Reaction equation

$$\text{THF} \longrightarrow \emptyset \tag{24}$$

Reactant

Table 27: Properties of each reactant.

Id	Name	SBO
THF	THF	

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{Henri\_Michaelis\_Menten\_\_irreversible\_\_1}\,(\mathrm{Km}, [\mathrm{THF}], \mathrm{V}) \quad (25)$$

$$\mathrm{Henri\_Michaelis\_Menten\_\_irreversible\_\_1}\,(\mathrm{Km}, [\mathrm{THF}], \mathrm{V}) = \frac{\mathrm{V} \cdot [\mathrm{THF}]}{\mathrm{Km} + [\mathrm{THF}]} \quad (26)$$

$$\mathrm{Henri\_Michaelis\_Menten\_\_irreversible\_\_1}\,(\mathrm{Km}, [\mathrm{THF}], \mathrm{V}) = \frac{\mathrm{V} \cdot [\mathrm{THF}]}{\mathrm{Km} + [\mathrm{THF}]} \quad (27)$$

Table 28: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Km	Km		$1.571 \cdot 10^{-4}$		☑
V	V		$1.243 \cdot 10^{-7}$		☑

6.10 Reaction CH2_THF_drain

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

Name CH2-THF_drain

Reaction equation

$$\mathrm{CH2\_THF} \longrightarrow \emptyset \quad (28)$$

Reactant

Table 29: Properties of each reactant.

Id	Name	SBO
CH2_THF	CH2-THF	

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{Henri\_Michaelis\_Menten\_\_irreversible\_\_2}\,([\mathrm{CH2\_THF}], \mathrm{Km}, \mathrm{V}) \quad (29)$$

$$\text{Henri\_Michaelis\_Menten\_\_irreversible\_\_2}([\text{CH2\_THF}], \text{Km}, \text{V}) = \frac{\text{V} \cdot [\text{CH2\_THF}]}{\text{Km} + [\text{CH2\_THF}]} \quad (30)$$

$$\text{Henri\_Michaelis\_Menten\_\_irreversible\_\_2}([\text{CH2\_THF}], \text{Km}, \text{V}) = \frac{\text{V} \cdot [\text{CH2\_THF}]}{\text{Km} + [\text{CH2\_THF}]} \quad (31)$$

Table 30: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
`Km`	Km		$5.921 \cdot 10^{-5}$		☑
`V`	V		$1.726 \cdot 10^{-7}$		☑

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 `H2_HMPt`

Name H2-HMPt

Notes `6-hydroxymethyldihydropterin`

Initial concentration $3.315 \cdot 10^{-6}$ mmol $\cdot$ ml^{-1}

This species takes part in three reactions (as a reactant in `FolK` and as a product in `PanB`, `H2-_HMPt_production`).

$$\frac{\text{d}}{\text{d}t}\text{H2\_HMPt} = v_6 + v_8 - v_1 \quad (32)$$

7.2 Species `ATP`

Name ATP

Initial concentration 0.0096 mmol $\cdot$ ml^{-1}

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ATP} = 0 \tag{33}$$

7.3 Species H2_HMPterinPP

Name H2-HMPterinPP

Notes 6-hydroxymethyldihydropterin

Initial concentration $10^{-5}\ \mathrm{mmol}\cdot\mathrm{ml}^{-1}$

This species takes part in two reactions (as a reactant in FolP and as a product in FolK).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{H2\_HMPterinPP} = v_1 - v_2 \tag{34}$$

7.4 Species AMP

Name AMP

Initial concentration $2.8\cdot 10^{-4}\ \mathrm{mmol}\cdot\mathrm{ml}^{-1}$

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

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

7.5 Species p_ABA

Name p-ABA

Initial concentration $10^{-5}\ \mathrm{mmol}\cdot\mathrm{ml}^{-1}$

This species takes part in three reactions (as a reactant in FolP and as a product in PanB, p_ABA-_production).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{p\_ABA} = v_6 + v_7 - v_2 \tag{36}$$

7.6 Species PPi

Name PPi

Initial concentration $5\cdot 10^{-4}\ \mathrm{mmol}\cdot\mathrm{ml}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{PPi} = 0 \tag{37}$$

7.7 Species H2_Pteroate

Name H2-Pteroate

Initial concentration $10^{-5}\ \mathrm{mmol}\cdot\mathrm{ml}^{-1}$

This species takes part in two reactions (as a reactant in FolC and as a product in FolP).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{H2\_Pteroate} = v_2 - v_3 \tag{38}$$

7.8 Species L_Glutamate

Name L-Glutamate

Initial concentration $8.46\cdot 10^{-4}\ \mathrm{mmol}\cdot\mathrm{ml}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{L\_Glutamate} = 0 \tag{39}$$

7.9 Species Phosphate

Name Phosphate

Initial concentration $0.01\ \mathrm{mmol}\cdot\mathrm{ml}^{-1}$

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

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

7.10 Species ADP

Name ADP

Initial concentration $5.6\cdot 10^{-4}\ \mathrm{mmol}\cdot\mathrm{ml}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ADP} = 0 \tag{41}$$

7.11 Species DHF

Name DHF

Initial concentration $10^{-5}\ \mathrm{mmol}\cdot\mathrm{ml}^{-1}$

This species takes part in two reactions (as a reactant in FolA and as a product in FolC).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{DHF} = v_3 - v_5 \tag{42}$$

7.12 Species L_serine

Name L-serine

Initial concentration $6.8\cdot 10^{-5}\ \mathrm{mmol}\cdot\mathrm{ml}^{-1}$

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

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

7.13 Species Glycine

Name Glycine

Initial concentration $2.77\cdot 10^{-4}\ \mathrm{mmol}\cdot\mathrm{ml}^{-1}$

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

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

7.14 Species NADP

Name NADP

Initial concentration $9.4\cdot 10^{-7}\ \mathrm{mmol}\cdot\mathrm{ml}^{-1}$

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

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

7.15 Species NADPH

Name NADPH

Initial concentration $9.4 \cdot 10^{-7}$ mmol $\cdot$ ml^{-1}

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{NADPH} = 0 \tag{46}$$

7.16 Species THF

Name THF

Initial concentration $1.69 \cdot 10^{-4}$ mmol $\cdot$ ml^{-1}

This species takes part in three reactions (as a reactant in GlyA, THF_drain and as a product in FolA).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{THF} = v_5 - v_4 - v_9 \tag{47}$$

7.17 Species CH2_THF

Name CH2-THF

Initial concentration $8.47 \cdot 10^{-5}$ mmol $\cdot$ ml^{-1}

This species takes part in three reactions (as a reactant in PanB, CH2_THF_drain and as a product in GlyA).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{CH2\_THF} = v_4 - v_6 - v_{10} \tag{48}$$

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.

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