

SBML Model Report

Model name: “Morrison1989_FolateCycle”



May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 1 format. This model was created by the following two authors: Nicolas Le Novre¹ and Tomas Radivoyevitch² at June 29th 2005 at 10:22 a. m. and last time modified at July fifth 2012 at 2:40 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	2
species types	0	species	33
events	0	constraints	0
reactions	47	function definitions	0
global parameters	1	unit definitions	2
rules	2	initial assignments	0

Model Notes

This is a folate model that includes folate polyglutamation.

Morrison and Allegra, JBC:264,10552-10566 (1989)

Folate cycle kinetics in breast cancer cells

Note: two flow BCs were converted into two downstream concentration BCs, thus removing the GAR and dUMP state variables.

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This dropped the number of ODEs from 21 to 19.

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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 `substance`

Name micromole (new default)

Notes Default unit of substance redefined to micromole by comparison with the article. Nicolas Le Novre

Definition μmol

2.2 Unit `time`

Name heure (new default)

Notes Default unit of time redefined to hour by comparison with the article. Nicolas Le Novre

Definition 3600 s

2.3 Unit `volume`

Notes Litre is the predefined SBML unit for volume.

Definition l

2.4 Unit `area`

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

Definition m^2

2.5 Unit `length`

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

Definition `m`

3 Compartments

This model contains two compartments.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
<code>ext</code>			3	1	litre	<input checked="" type="checkbox"/>	
<code>cell</code>			3	1	litre	<input checked="" type="checkbox"/>	<code>ext</code>

3.1 Compartment `ext`

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

3.2 Compartment `cell`

This is a three dimensional compartment with a constant size of one litre, which is surrounded by `ext`.

4 Species

This model contains 33 species. The boundary condition of 13 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
FH2f	dihydrofolate free	cell	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
FH2b	dihydrofolate bound	cell	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input checked="" type="checkbox"/>
DHFRf	dihydrofolate reductase free	cell	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
DHFRtot	dihydrofolate reductase total	cell	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input checked="" type="checkbox"/>
FH4	tetrahydrofolate	cell	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
CH2FH4	5,10-methylene-tetrahydrofolate	cell	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
CH3FH4	5-methyl-tetrahydrofolate	cell	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
CHOFH4	10-formyl-tetrahydrofolate	cell	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
FFH2	10-formyl-dihydrofolate	cell	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
HCHO		cell	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
FGAR		cell	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
AICAR		cell	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
MTX1		cell	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
MTX2		cell	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
MTX3		cell	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
MTX4		cell	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
MTX5		cell	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
MTX1b		cell	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
MTX2b		cell	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
MTX3b		cell	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
MTX4b		cell	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>

Id	Name	Compartment	Derived Unit	Constant	Boundary Condi- tion
MTX5b		cell	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input type="checkbox"/>
EMTX		ext	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input checked="" type="checkbox"/>
dUMP		cell	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input checked="" type="checkbox"/>
GAR		cell	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input checked="" type="checkbox"/>
serine		cell	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input checked="" type="checkbox"/>
formate		cell	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input checked="" type="checkbox"/>
ATP		cell	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input checked="" type="checkbox"/>
glutamine		cell	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input checked="" type="checkbox"/>
glycine		cell	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input checked="" type="checkbox"/>
NADP		cell	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input checked="" type="checkbox"/>
NADPH		cell	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input checked="" type="checkbox"/>
homocysteine		cell	$\mu\text{mol} \cdot \text{l}^{-1}$	<input type="checkbox"/>	<input checked="" type="checkbox"/>

5 Parameter

This model contains one global parameter.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Keq			0.32		<input checked="" type="checkbox"/>

6 Rules

This is an overview of two rules.

6.1 Rule FH2b

Rule FH2b is an assignment rule for species FH2b:

$$\text{FH2b} = \frac{[\text{FH2f}] \cdot [\text{DHFRf}]}{\text{Keq}} \quad (1)$$

6.2 Rule DHFRtot

Rule DHFRtot is an assignment rule for species DHFRtot:

$$\text{DHFRtot} = [\text{FH2b}] + [\text{DHFRf}] + [\text{MTX1b}] + [\text{MTX2b}] + [\text{MTX3b}] + [\text{MTX4b}] + [\text{MTX5b}] \quad (2)$$

Derived unit $\mu\text{mol} \cdot \text{l}^{-1}$

7 Reactions

This model contains 47 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

Nº	Id	Name	Reaction Equation	SBO
1	SHMT		$\text{FH4} + \text{serine} \longrightarrow \text{CH2FH4}$	
2	SHMT _r		$\text{CH2FH4} \xrightarrow{\text{glycine}} \text{FH4}$	
3	HCHO _{to} CH2FH4		$\text{FH4} + \text{HCHO} \longrightarrow \text{CH2FH4}$	
4	CH2FH4 _{to} HCHO		$\text{CH2FH4} \longrightarrow \text{FH4} + \text{HCHO}$	
5	MTHFR		$\text{CH2FH4} + \text{NADPH} \xrightarrow{\text{FH2f, MTX1, MTX2, MTX3, MTX4, MTX5}} \text{CH3FH4}$	
6	MTR		$\text{CH3FH4} + \text{homocysteine} \longrightarrow \text{FH4}$	
7	HCOOH _{to} CHOFH4		$\text{FH4} + \text{formate} + \text{ATP} \longrightarrow \text{CHOFH4}$	
8	GARFT		$\text{CHOFH4} + \text{GAR} \xrightarrow{\text{FH2f, FFH2, MTX1, MTX2, MTX3, MTX4, MTX5}} \text{FGAR} + \text{FH4}$	
9	ATIC7		$\text{CHOFH4} + \text{AICAR} \xrightarrow{\text{FH2f, FFH2, MTX1, MTX2, MTX3, MTX4, MTX5}} \text{FH4}$	
10	MTHFD		$\text{CH2FH4} + \text{NADP} \longrightarrow \text{CHOFH4}$	
11	TYMS		$\text{CH2FH4} + \text{dUMP} \xrightarrow{\text{FH2f, FFH2, MTX1, MTX2, MTX3, MTX4, MTX5}} \text{FH2f}$	
12	DHFReductase		$\text{FH2f} \xrightarrow{\text{FH2b}} \text{FH4}$	
13	FFH2syn		$\text{FH2f} \longrightarrow \text{FFH2}$	
14	ATIC12		$\text{FFH2} + \text{AICAR} \xrightarrow{\text{FH2f, MTX1, MTX2, MTX3, MTX4, MTX5}} \text{FH2f}$	
15	AICARsyn		$\text{FGAR} \xrightarrow{\text{glutamine}} \text{AICAR}$	
16	FPGS12		$\text{MTX1} \longrightarrow \text{MTX2}$	
17	FPGS23		$\text{MTX2} \longrightarrow \text{MTX3}$	
18	FPGS34		$\text{MTX3} \longrightarrow \text{MTX4}$	

Nº	Id	Name	Reaction Equation	SBO
19	FPGS45		$\text{MTX4} \longrightarrow \text{MTX5}$	
20	GGH21		$\text{MTX2} \longrightarrow \text{MTX1}$	
21	GGH32		$\text{MTX3} \longrightarrow \text{MTX2}$	
22	GGH43		$\text{MTX4} \longrightarrow \text{MTX3}$	
23	GGH54		$\text{MTX5} \longrightarrow \text{MTX4}$	
24	RFC		$\text{EMTX} \longrightarrow \text{MTX1}$	
25	MTX1export		$\text{MTX1} \longrightarrow \emptyset$	
26	MTX2export		$\text{MTX2} \longrightarrow \emptyset$	
27	MTX3export		$\text{MTX3} \longrightarrow \emptyset$	
28	MTX4export		$\text{MTX4} \longrightarrow \emptyset$	
29	MTX5export		$\text{MTX5} \longrightarrow \emptyset$	
30	MTX1on		$\text{MTX1} + \text{DHFRf} \longrightarrow \text{MTX1b}$	
31	MTX2on		$\text{MTX2} + \text{DHFRf} \longrightarrow \text{MTX2b}$	
32	MTX3on		$\text{MTX3} + \text{DHFRf} \longrightarrow \text{MTX3b}$	
33	MTX4on		$\text{MTX4} + \text{DHFRf} \longrightarrow \text{MTX4b}$	
34	MTX5on		$\text{MTX5} + \text{DHFRf} \longrightarrow \text{MTX5b}$	
35	MTX1off		$\text{MTX1b} \longrightarrow \text{MTX1} + \text{DHFRf}$	
36	MTX2off		$\text{MTX2b} \longrightarrow \text{MTX2} + \text{DHFRf}$	
37	MTX3off		$\text{MTX3b} \longrightarrow \text{MTX3} + \text{DHFRf}$	
38	MTX4off		$\text{MTX4b} \longrightarrow \text{MTX4} + \text{DHFRf}$	
39	MTX5off		$\text{MTX5b} \longrightarrow \text{MTX5} + \text{DHFRf}$	
40	DHFRfsyn		$\emptyset \xrightarrow{\text{EMTX}} \text{DHFRf}$	
41	DHFRdeg		$\text{DHFRf} \xrightarrow{\text{FH2b}} \emptyset$	
42	FH2bdeg		$\emptyset \xrightarrow{\text{FH2b}} \text{FH2f}$	
43	MTX1deg		$\text{MTX1b} \longrightarrow \text{MTX1}$	
44	MTX2deg		$\text{MTX2b} \longrightarrow \text{MTX2}$	
45	MTX3deg		$\text{MTX3b} \longrightarrow \text{MTX3}$	
46	MTX4deg		$\text{MTX4b} \longrightarrow \text{MTX4}$	

Nº	Id	Name	Reaction Equation	SBO
47	MTX5deg		$\text{MTX5b} \longrightarrow \text{MTX5}$	

7.1 Reaction SHMT

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

Reaction equation



Reactants

Table 6: Properties of each reactant.

Id	Name	SBO
FH4	tetrahydrofolate	
serine		

Product

Table 7: Properties of each product.

Id	Name	SBO
CH2FH4	5,10-methylene-tetrahydrofolate	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \text{vol}(\text{cell}) \cdot \frac{V_m \cdot \frac{\frac{[\text{serine}]}{K_{m2}}}{1 + \frac{[\text{serine}]}{K_{m2}}} \cdot \frac{[\text{FH4}]}{K_{m1}}}{1 + \frac{[\text{FH4}]}{K_{m1}}} \quad (4)$$

Table 8: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vm			18330.0		<input checked="" type="checkbox"/>
Km1			1.7		<input checked="" type="checkbox"/>
Km2			210.0		<input checked="" type="checkbox"/>

7.2 Reaction SHMT_r

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

Reaction equation



Reactant

Table 9: Properties of each reactant.

Id	Name	SBO
CH2FH4	5,10-methylene-tetrahydrofolate	

Modifier

Table 10: Properties of each modifier.

Id	Name	SBO
	glycine	

Product

Table 11: Properties of each product.

Id	Name	SBO
FH4	tetrahydrofolate	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \text{vol}(\text{cell}) \cdot \frac{V_m \cdot \frac{[\text{glycine}]}{K_{m2}} \cdot \frac{[\text{CH}_2\text{FH}_4]}{K_{m1}}}{1 + \frac{[\text{glycine}]}{K_{m2}} + \frac{[\text{CH}_2\text{FH}_4]}{K_{m1}}} \quad (6)$$

Table 12: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vm			$1.22 \cdot 10^7$		✓
Km1			3200.000		✓
Km2			10000.000		✓

7.3 Reaction $\text{HCHO} \rightarrow \text{CH}_2\text{FH}_4$

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

Reaction equation



Reactants

Table 13: Properties of each reactant.

Id	Name	SBO
FH4	tetrahydrofolate	
HCHO		

Product

Table 14: Properties of each product.

Id	Name	SBO
CH ₂ FH ₄	5,10-methylene-tetrahydrofolate	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \text{vol}(\text{cell}) \cdot \text{hp} \cdot [\text{FH}_4] \cdot [\text{HCHO}] \quad (8)$$

Table 15: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
hp			23.2		<input checked="" type="checkbox"/>

7.4 Reaction $\text{CH}_2\text{FH}_4 \rightarrow \text{HCHO}$

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

Reaction equation



Reactant

Table 16: Properties of each reactant.

Id	Name	SBO
CH2FH4	5,10-methylene-tetrahydrofolate	

Products

Table 17: Properties of each product.

Id	Name	SBO
FH4	tetrahydrofolate	
HCHO		

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \text{vol}(\text{cell}) \cdot h1 \cdot [\text{CH2FH4}] \quad (10)$$

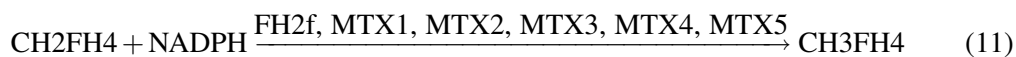
Table 18: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
h1			0.3		<input checked="" type="checkbox"/>

7.5 Reaction MTHFR

This is an irreversible reaction of two reactants forming one product influenced by six modifiers.

Reaction equation



Reactants

Table 19: Properties of each reactant.

Id	Name	SBO
CH2FH4	5,10-methylene-tetrahydrofolate	

Id	Name	SBO
NADPH		

Modifiers

Table 20: Properties of each modifier.

Id	Name	SBO
FH2f	dihydrofolate free	
MTX1		
MTX2		
MTX3		
MTX4		
MTX5		

Product

Table 21: Properties of each product.

Id	Name	SBO
CH3FH4	5-methyl-tetrahydrofolate	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \text{vol}(\text{cell}) \quad (12)$$

$$\frac{V_m \cdot [\text{CH}_2\text{FH}_4] \cdot [\text{NADPH}]}{[\text{NADPH}] \cdot [\text{CH}_2\text{FH}_4] + [\text{CH}_2\text{FH}_4] \cdot K_{m2} + ([\text{NADPH}] + K_{m2}) \cdot K_{m1} \cdot \left(1 + \frac{[\text{MTX1}]}{K_{i21}} + \frac{[\text{MTX2}]}{K_{i22}} + \frac{[\text{MTX3}]}{K_{i23}} + \frac{[\text{MTX4}]}{K_{i24}} + \frac{[\text{MTX5}]}{K_{i25}}\right)}$$

Table 22: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vm			224.80		✓
Km1			50.00		✓
Km2			50.00		✓
Ki1			0.40		✓
Ki21			59.00		✓
Ki22			21.30		✓
Ki23			7.68		✓

Id	Name	SBO	Value	Unit	Constant
Ki24			2.77		<input checked="" type="checkbox"/>
Ki25			1.00		<input checked="" type="checkbox"/>

7.6 Reaction MTR

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

Reaction equation



Reactants

Table 23: Properties of each reactant.

Id	Name	SBO
CH3FH4	5-methyl-tetrahydrofolate	
homocysteine		

Product

Table 24: Properties of each product.

Id	Name	SBO
FH4	tetrahydrofolate	

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \text{vol}(\text{cell}) \cdot \frac{V_m \cdot \frac{\frac{[\text{homocysteine}]}{K_{m2}}}{1 + \frac{[\text{homocysteine}]}{K_{m2}}} \cdot \frac{[\text{CH3FH4}]}{K_{m1}}}{1 + \frac{[\text{CH3FH4}]}{K_{m1}}} \quad (14)$$

Table 25: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vm			22600.0		<input checked="" type="checkbox"/>
Km1			125.0		<input checked="" type="checkbox"/>
Km2			2900.0		<input checked="" type="checkbox"/>

7.7 Reaction $\text{HCOOH} \rightarrow \text{CHO FH}_4$

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

Reaction equation



Reactants

Table 26: Properties of each reactant.

Id	Name	SBO
FH4	tetrahydrofolate	
formate		
ATP		

Product

Table 27: Properties of each product.

Id	Name	SBO
CHO FH4	10-formyl-tetrahydrofolate	

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \text{vol}(\text{cell}) \cdot \frac{V_m}{\left(1 + \frac{K_{m1}}{[\text{FH}_4]}\right) \cdot \left(1 + \frac{K_{m2}}{[\text{ATP}]}\right) \cdot \left(1 + \frac{K_{m3}}{[\text{formate}]}\right)} \quad (16)$$

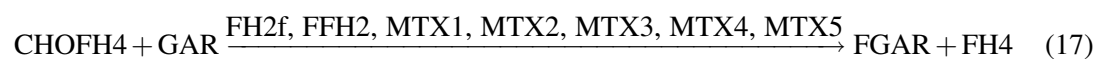
Table 28: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vm			3600.0		<input checked="" type="checkbox"/>
Km1			230.0		<input checked="" type="checkbox"/>
Km2			56.0		<input checked="" type="checkbox"/>
Km3			1600.0		<input checked="" type="checkbox"/>

7.8 Reaction GARFT

This is an irreversible reaction of two reactants forming two products influenced by seven modifiers.

Reaction equation



Reactants

Table 29: Properties of each reactant.

Id	Name	SBO
CHOFH4	10-formyl-tetrahydrofolate	
GAR		

Modifiers

Table 30: Properties of each modifier.

Id	Name	SBO
FH2f	dihydrofolate free	
FFH2	10-formyl-dihydrofolate	
MTX1		
MTX2		
MTX3		
MTX4		
MTX5		

Products

Table 31: Properties of each product.

Id	Name	SBO
FGAR		
FH4	tetrahydrofolate	

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \text{vol}(\text{cell}) \quad (18)$$

$$\frac{V_m \cdot [\text{CHOFH4}] \cdot [\text{GAR}]}{[\text{GAR}] \cdot [\text{CHOFH4}] + [\text{CHOFH4}] \cdot K_{m2} + ([\text{GAR}] + K_{m2}) \cdot K_{m1} \cdot \left(1 + \frac{[\text{MTX1}]}{K_{i21}} + \frac{[\text{MTX2}]}{K_{i22}} + \frac{[\text{MTX3}]}{K_{i23}} + \frac{[\text{MTX4}]}{K_{i24}} + \frac{[\text{MTX5}]}{K_{i25}}\right)}$$

Table 32: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vm			4126.0		<input checked="" type="checkbox"/>
Km1			4.9		<input checked="" type="checkbox"/>
Km2			52.0		<input checked="" type="checkbox"/>
Ki1			5.0		<input checked="" type="checkbox"/>
Ki1f			1.0		<input checked="" type="checkbox"/>
Ki21			84.0		<input checked="" type="checkbox"/>
Ki22			60.0		<input checked="" type="checkbox"/>
Ki23			43.0		<input checked="" type="checkbox"/>
Ki24			31.0		<input checked="" type="checkbox"/>
Ki25			22.0		<input checked="" type="checkbox"/>

7.9 Reaction ATIC7

This is an irreversible reaction of two reactants forming one product influenced by seven modifiers.

Reaction equation



Reactants

Table 33: Properties of each reactant.

Id	Name	SBO
CHOFH4	10-formyl-tetrahydrofolate	
AICAR		

Modifiers

Table 34: Properties of each modifier.

Id	Name	SBO
FH2f	dihydrofolate free	
FFH2	10-formyl-dihydrofolate	
MTX1		
MTX2		
MTX3		
MTX4		
MTX5		

Product

Table 35: Properties of each product.

Id	Name	SBO
FH4	tetrahydrofolate	

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \text{vol}(\text{cell}) \quad (20)$$

$$\frac{V_m \cdot [\text{CHOFH4}] \cdot [\text{AICAR}]}{[\text{AICAR}] \cdot [\text{CHOFH4}] + [\text{CHOFH4}] \cdot K_{m2} + ([\text{AICAR}] + K_{m2}) \cdot K_{m1} \cdot \left(1 + \frac{[\text{MTX1}]}{K_{i21}} + \frac{[\text{MTX2}]}{K_{i22}} + \frac{[\text{MTX3}]}{K_{i23}} + \frac{[\text{MTX4}]}{K_{i24}} + \frac{[\text{MTX5}]}{K_{i25}}\right)}$$

Table 36: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vm			31675.00		✓
Km1			5.50		✓
Km2			24.00		✓
Ki1			2.89		✓
Ki1f			5.30		✓
Ki21			40.00		✓
Ki22			31.50		✓
Ki23			2.33		✓
Ki24			3.61		✓
Ki25			5.89		✓

7.10 Reaction MTHFD

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

Reaction equation



Reactants

Table 37: Properties of each reactant.

Id	Name	SBO
CH2FH4	5,10-methylene-tetrahydrofolate	
NADP		

Product

Table 38: Properties of each product.

Id	Name	SBO
CHOFH4	10-formyl-tetrahydrofolate	

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = \text{vol}(\text{cell}) \cdot V_m \cdot \frac{\frac{[\text{CH}_2\text{FH}_4]}{K_{m1}}}{1 + \frac{[\text{CH}_2\text{FH}_4]}{K_{m1}}} \cdot \frac{\frac{[\text{NADP}]}{K_{m2}}}{1 + \frac{[\text{NADP}]}{K_{m2}}} \quad (22)$$

Table 39: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vm			68500.0		<input checked="" type="checkbox"/>
Km1			3.0		<input checked="" type="checkbox"/>
Km2			21.8		<input checked="" type="checkbox"/>

7.11 Reaction TYMS

This is an irreversible reaction of two reactants forming one product influenced by seven modifiers.

Reaction equation



Reactants

Table 40: Properties of each reactant.

Id	Name	SBO
CH2FH4	5,10-methylene-tetrahydrofolate	
dUMP		

Modifiers

Table 41: Properties of each modifier.

Id	Name	SBO
FH2f	dihydrofolate free	
FFH2	10-formyl-dihydrofolate	
MTX1		
MTX2		
MTX3		
MTX4		
MTX5		

Product

Table 42: Properties of each product.

Id	Name	SBO
FH2f	dihydrofolate free	

Kinetic Law

Derived unit contains undeclared units

$$v_{11} = \text{vol}(\text{cell}) \quad (24)$$

$$[dUMP] \cdot [CH_2FH_4] \cdot \left(1 + \frac{[MTX1]}{Ki21} + \frac{[MTX2]}{Ki22} + \frac{[MTX3]}{Ki23} + \frac{[MTX4]}{Ki24} + \frac{[MTX5]}{Ki25} + \frac{[FH2f]}{Ki1} \right) + Km1 \cdot [dUMP] \cdot \left(\frac{[FFH2]}{Ki1f} \right) \cdot$$

Table 43: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vm			58.000		✓
Km1			2.500		✓
Km2			1.800		✓
Ki1			3.000		✓
Ki1f			1.600		✓
Ki21			13.000		✓
Ki22			0.080		✓
Ki23			0.070		✓
Ki24			0.065		✓
Ki25			0.047		✓

7.12 Reaction DHFReductase

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

Reaction equation



Reactant

Table 44: Properties of each reactant.

Id	Name	SBO
FH2f	dihydrofolate free	

Modifier

Table 45: Properties of each modifier.

Id	Name	SBO
FH2b	dihydrofolate bound	

Product

Table 46: Properties of each product.

Id	Name	SBO
FH4	tetrahydrofolate	

Kinetic Law

Derived unit contains undeclared units

$$v_{12} = \text{vol}(\text{cell}) \cdot k_{\text{ter}} \cdot [\text{FH2b}] \quad (26)$$

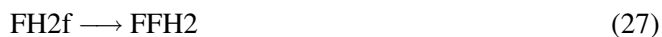
Table 47: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k _{ter}			2109.4		<input checked="" type="checkbox"/>

7.13 Reaction FFH2syn

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

Reaction equation



Reactant

Table 48: Properties of each reactant.

Id	Name	SBO
FH2f	dihydrofolate free	

Product

Table 49: Properties of each product.

Id	Name	SBO
FFH2	10-formyl-dihydrofolate	

Kinetic Law

Derived unit contains undeclared units

$$v_{13} = \text{vol}(\text{cell}) \cdot V_m \cdot [\text{FH2f}] \quad (28)$$

Table 50: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V _m			65.0		<input checked="" type="checkbox"/>

7.14 Reaction ATIC12

This is an irreversible reaction of two reactants forming one product influenced by six modifiers.

Reaction equation



Reactants

Table 51: Properties of each reactant.

Id	Name	SBO
FFH2	10-formyl-dihydrofolate	
AICAR		

Modifiers

Table 52: Properties of each modifier.

Id	Name	SBO
FH2f	dihydrofolate free	
MTX1		
MTX2		
MTX3		
MTX4		
MTX5		

Product

Table 53: Properties of each product.

Id	Name	SBO
FH2f	dihydrofolate free	

Kinetic Law

Derived unit contains undeclared units

$$v_{14} = \text{vol}(\text{cell}) \cdot \frac{V_m \cdot [\text{FFH2}] \cdot [\text{AICAR}]}{[\text{AICAR}] \cdot [\text{FFH2}] + [\text{FFH2}] \cdot K_{m2} + ([\text{AICAR}] + K_{m2}) \cdot K_{m1} \cdot \left(1 + \frac{[\text{MTX1}]}{K_{i21}} + \frac{[\text{MTX2}]}{K_{i22}} + \frac{[\text{MTX3}]}{K_{i23}} + \frac{[\text{MTX4}]}{K_{i24}} + \frac{[\text{MTX5}]}{K_{i25}}\right)}$$

(30)

Table 54: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vm			9503.00		<input checked="" type="checkbox"/>
Km1			5.30		<input checked="" type="checkbox"/>
Km2			24.00		<input checked="" type="checkbox"/>
Ki1			2.89		<input checked="" type="checkbox"/>
Ki1f			5.50		<input checked="" type="checkbox"/>
Ki21			40.00		<input checked="" type="checkbox"/>
Ki22			31.50		<input checked="" type="checkbox"/>
Ki23			2.33		<input checked="" type="checkbox"/>
Ki24			3.61		<input checked="" type="checkbox"/>
Ki25			5.89		<input checked="" type="checkbox"/>

7.15 Reaction AICARsyn

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

Reaction equation



Reactant

Table 55: Properties of each reactant.

Id	Name	SBO
FGAR		

Id	Name	SBO
----	------	-----

Modifier

Table 56: Properties of each modifier.

Id	Name	SBO
	glutamine	

Product

Table 57: Properties of each product.

Id	Name	SBO
	AICAR	

Kinetic Law

Derived unit contains undeclared units

$$v_{15} = \text{vol}(\text{cell}) \cdot V_m \cdot \frac{\frac{[\text{glutamine}]}{K_{m1}}}{1 + \frac{[\text{glutamine}]}{K_{m1}}} \cdot \frac{\frac{[\text{FGAR}]}{K_{m2}}}{1 + \frac{[\text{FGAR}]}{K_{m2}}} \quad (32)$$

Table 58: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vm			4656.0		<input checked="" type="checkbox"/>
Km1			100.0		<input checked="" type="checkbox"/>
Km2			100.0		<input checked="" type="checkbox"/>

7.16 Reaction FPGS12

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

Reaction equation



Reactant

Table 59: Properties of each reactant.

Id	Name	SBO
MTX1		

Product

Table 60: Properties of each product.

Id	Name	SBO
MTX2		

Kinetic Law

Derived unit contains undeclared units

$$v_{16} = \text{vol}(\text{cell}) \cdot V_m \cdot [\text{MTX1}] \quad (34)$$

Table 61: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V _m			0.129		<input checked="" type="checkbox"/>

7.17 Reaction FPGS23

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

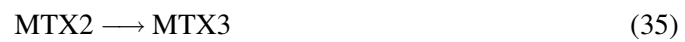
Reaction equation**Reactant**

Table 62: Properties of each reactant.

Id	Name	SBO
MTX2		

Product

Table 63: Properties of each product.

Id	Name	SBO
MTX3		

Kinetic Law**Derived unit** contains undeclared units

$$v_{17} = \text{vol}(\text{cell}) \cdot V_m \cdot [\text{MTX2}] \quad (36)$$

Table 64: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V _m			0.369		<input checked="" type="checkbox"/>

7.18 Reaction FPGS34

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

Reaction equation**Reactant**

Table 65: Properties of each reactant.

Id	Name	SBO
MTX3		

Product

Table 66: Properties of each product.

Id	Name	SBO
MTX4		

Kinetic Law**Derived unit** contains undeclared units

$$v_{18} = \text{vol}(\text{cell}) \cdot V_m \cdot [\text{MTX3}] \quad (38)$$

Table 67: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V _m			0.118		<input checked="" type="checkbox"/>

7.19 Reaction FPGS45

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

Reaction equation



Reactant

Table 68: Properties of each reactant.

Id	Name	SBO
MTX4		

Product

Table 69: Properties of each product.

Id	Name	SBO
MTX5		

Kinetic Law

Derived unit contains undeclared units

$$v_{19} = \text{vol}(\text{cell}) \cdot V_m \cdot [\text{MTX4}] \quad (40)$$

Table 70: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V _m			0.185		<input checked="" type="checkbox"/>

7.20 Reaction GGH21

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

Reaction equation



Reactant

Table 71: Properties of each reactant.

Id	Name	SBO
MTX2		

Product

Table 72: Properties of each product.

Id	Name	SBO
MTX1		

Kinetic Law

Derived unit contains undeclared units

$$v_{20} = \text{vol}(\text{cell}) \cdot V_m \cdot [\text{MTX2}] \quad (42)$$

Table 73: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V _m			0.195		<input checked="" type="checkbox"/>

7.21 Reaction GGH32

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

Reaction equation



Reactant

Table 74: Properties of each reactant.

Id	Name	SBO
MTX3		

Product

Table 75: Properties of each product.

Id	Name	SBO
MTX2		

Kinetic Law

Derived unit contains undeclared units

$$v_{21} = \text{vol}(\text{cell}) \cdot V_m \cdot [\text{MTX3}] \quad (44)$$

Table 76: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V _m			0.025		<input checked="" type="checkbox"/>

7.22 Reaction GGH43

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

Reaction equation



Reactant

Table 77: Properties of each reactant.

Id	Name	SBO
MTX4		

Product

Table 78: Properties of each product.

Id	Name	SBO
MTX3		

Kinetic Law

Derived unit contains undeclared units

$$v_{22} = \text{vol}(\text{cell}) \cdot V_m \cdot [\text{MTX4}] \quad (46)$$

Table 79: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V _m			0.031		<input checked="" type="checkbox"/>

7.23 Reaction GGH54

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

Reaction equation



Reactant

Table 80: Properties of each reactant.

Id	Name	SBO
MTX5		

Product

Table 81: Properties of each product.

Id	Name	SBO
MTX4		

Kinetic Law

Derived unit contains undeclared units

$$v_{23} = \text{vol}(\text{cell}) \cdot V_m \cdot [\text{MTX5}] \quad (48)$$

Table 82: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vm			0.191		<input checked="" type="checkbox"/>

7.24 Reaction RFC

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

Reaction equation



Reactant

Table 83: Properties of each reactant.

Id	Name	SBO
EMTX		

Product

Table 84: Properties of each product.

Id	Name	SBO
MTX1		

Kinetic Law

Derived unit contains undeclared units

$$v_{24} = \text{vol}(\text{ext}) \cdot \frac{V_m \cdot [\text{EMTX}]}{K_m + [\text{EMTX}]} \quad (50)$$

Table 85: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vm			82.2		<input checked="" type="checkbox"/>
Km			8.2		<input checked="" type="checkbox"/>

7.25 Reaction MTX1export

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

Reaction equation



Reactant

Table 86: Properties of each reactant.

Id	Name	SBO
MTX1		

Kinetic Law

Derived unit contains undeclared units

$$v_{25} = \text{vol}(\text{cell}) \cdot V_m \cdot [\text{MTX1}] \quad (52)$$

Table 87: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vm			4.65		<input checked="" type="checkbox"/>

7.26 Reaction MTX2export

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

Reaction equation



Reactant

Table 88: Properties of each reactant.

Id	Name	SBO
MTX2		

Kinetic Law**Derived unit** contains undeclared units

$$v_{26} = \text{vol}(\text{cell}) \cdot V_m \cdot [\text{MTX2}] \quad (54)$$

Table 89: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V _m			0.0		<input checked="" type="checkbox"/>

7.27 Reaction `MTX3export`

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

Reaction equation**Reactant**

Table 90: Properties of each reactant.

Id	Name	SBO
MTX3		

Kinetic Law**Derived unit** contains undeclared units

$$v_{27} = \text{vol}(\text{cell}) \cdot V_m \cdot [\text{MTX3}] \quad (56)$$

Table 91: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V _m			0.063		<input checked="" type="checkbox"/>

7.28 Reaction MTX4_{export}

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

Reaction equation



Reactant

Table 92: Properties of each reactant.

Id	Name	SBO
MTX4		

Kinetic Law

Derived unit contains undeclared units

$$v_{28} = \text{vol}(\text{cell}) \cdot V_m \cdot [\text{MTX4}] \quad (58)$$

Table 93: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V _m			0.063		<input checked="" type="checkbox"/>

7.29 Reaction MTX5_{export}

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

Reaction equation



Reactant

Table 94: Properties of each reactant.

Id	Name	SBO
MTX5		

Kinetic Law

Derived unit contains undeclared units

$$v_{29} = \text{vol}(\text{cell}) \cdot V_m \cdot [\text{MTX5}] \quad (60)$$

Table 95: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V _m			0.063		<input checked="" type="checkbox"/>

7.30 Reaction MTX1on

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

Reaction equation



Reactants

Table 96: Properties of each reactant.

Id	Name	SBO
MTX1		
DHFRf	dihydrofolate reductase free	

Product

Table 97: Properties of each product.

Id	Name	SBO
MTX1b		

Kinetic Law

Derived unit contains undeclared units

$$v_{30} = \text{vol}(\text{cell}) \cdot V_m \cdot [\text{DHFRf}] \cdot [\text{MTX1}] \quad (62)$$

Table 98: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V _m			23100.0		<input checked="" type="checkbox"/>

7.31 Reaction MTX2on

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

Reaction equation



Reactants

Table 99: Properties of each reactant.

Id	Name	SBO
MTX2		
DHFRf	dihydrofolate reductase free	

Product

Table 100: Properties of each product.

Id	Name	SBO
MTX2b		

Kinetic Law

Derived unit contains undeclared units

$$v_{31} = \text{vol}(\text{cell}) \cdot V_m \cdot [\text{DHFRf}] \cdot [\text{MTX2}] \quad (64)$$

Table 101: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V _m			44300.0		<input checked="" type="checkbox"/>

7.32 Reaction MTX3on

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

Reaction equation



Reactants

Table 102: Properties of each reactant.

Id	Name	SBO
MTX3		
DHFRf	dihydrofolate reductase free	

Product

Table 103: Properties of each product.

Id	Name	SBO
MTX3b		

Kinetic Law

Derived unit contains undeclared units

$$v_{32} = \text{vol}(\text{cell}) \cdot V_m \cdot [\text{DHFRf}] \cdot [\text{MTX3}] \quad (66)$$

Table 104: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V _m			85100.0		<input checked="" type="checkbox"/>

7.33 Reaction MTX4on

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

Reaction equation



Reactants

Table 105: Properties of each reactant.

Id	Name	SBO
MTX4		
DHFRf	dihydrofolate reductase free	

Product

Table 106: Properties of each product.

Id	Name	SBO
MTX4b		

Kinetic Law

Derived unit contains undeclared units

$$v_{33} = \text{vol}(\text{cell}) \cdot V_m \cdot [\text{DHFRf}] \cdot [\text{MTX4}] \quad (68)$$

Table 107: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V _m			163000.0		<input checked="" type="checkbox"/>

7.34 Reaction MTX5on

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

Reaction equation



Reactants

Table 108: Properties of each reactant.

Id	Name	SBO
MTX5		

Id	Name	SBO
DHFRf	dihydrofolate reductase free	

Product

Table 109: Properties of each product.

Id	Name	SBO
MTX5b		

Kinetic Law

Derived unit contains undeclared units

$$v_{34} = \text{vol}(\text{cell}) \cdot V_m \cdot [\text{DHFRf}] \cdot [\text{MTX5}] \quad (70)$$

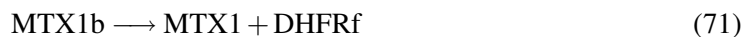
Table 110: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V _m			314000.0		<input checked="" type="checkbox"/>

7.35 Reaction MTX1off

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

Reaction equation



Reactant

Table 111: Properties of each reactant.

Id	Name	SBO
MTX1b		

Products

Table 112: Properties of each product.

Id	Name	SBO
MTX1		
DHFRf	dihydrofolate reductase free	

Kinetic Law

Derived unit contains undeclared units

$$v_{35} = \text{vol}(\text{cell}) \cdot V_m \cdot [\text{MTX1b}] \quad (72)$$

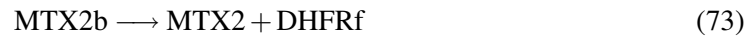
Table 113: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V _m			0.42		<input checked="" type="checkbox"/>

7.36 Reaction MTX2off

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

Reaction equation



Reactant

Table 114: Properties of each reactant.

Id	Name	SBO
MTX2b		

Products

Table 115: Properties of each product.

Id	Name	SBO
MTX2		
DHFRf	dihydrofolate reductase free	

Kinetic Law

Derived unit contains undeclared units

$$v_{36} = \text{vol}(\text{cell}) \cdot V_m \cdot [\text{MTX2b}] \quad (74)$$

Table 116: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V _m			0.42		<input checked="" type="checkbox"/>

7.37 Reaction MTX3off

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

Reaction equation



Reactant

Table 117: Properties of each reactant.

Id	Name	SBO
MTX3b		

Products

Table 118: Properties of each product.

Id	Name	SBO
MTX3		
DHFRf	dihydrofolate reductase free	

Kinetic Law

Derived unit contains undeclared units

$$v_{37} = \text{vol}(\text{cell}) \cdot V_m \cdot [\text{MTX3b}] \quad (76)$$

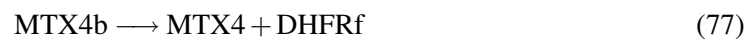
Table 119: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V _m			0.42		<input checked="" type="checkbox"/>

7.38 Reaction *MTX4off*

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

Reaction equation



Reactant

Table 120: Properties of each reactant.

Id	Name	SBO
MTX4b		

Products

Table 121: Properties of each product.

Id	Name	SBO
MTX4		
DHFRf	dihydrofolate reductase free	

Kinetic Law

Derived unit contains undeclared units

$$v_{38} = \text{vol}(\text{cell}) \cdot V_m \cdot [\text{MTX4b}] \quad (78)$$

Table 122: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V _m			0.42		<input checked="" type="checkbox"/>

7.39 Reaction MTX5off

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

Reaction equation



Reactant

Table 123: Properties of each reactant.

Id	Name	SBO
MTX5b		

Products

Table 124: Properties of each product.

Id	Name	SBO
MTX5		
DHFRf	dihydrofolate reductase free	

Kinetic Law

Derived unit contains undeclared units

$$v_{39} = \text{vol}(\text{cell}) \cdot V_m \cdot [\text{MTX5b}] \quad (80)$$

Table 125: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V _m			0.42		<input checked="" type="checkbox"/>

7.40 Reaction DHFRfsyn

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

Reaction equation



Modifier

Table 126: Properties of each modifier.

Id	Name	SBO
EMTX		

Product

Table 127: Properties of each product.

Id	Name	SBO
DHFRf	dihydrofolate reductase free	

Kinetic Law

Derived unit contains undeclared units

$$v_{40} = \text{vol}(\text{cell}) \cdot (k_0 + k_1 \cdot [\text{EMTX}]) \quad (82)$$

Table 128: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k0			0.019		<input checked="" type="checkbox"/>
k1			0.044		<input checked="" type="checkbox"/>

7.41 Reaction DHFRdeg

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

Reaction equation



Reactant

Table 129: Properties of each reactant.

Id	Name	SBO
DHFRf	dihydrofolate reductase free	

Modifier

Table 130: Properties of each modifier.

Id	Name	SBO
FH2b	dihydrofolate bound	

Kinetic Law

Derived unit contains undeclared units

$$v_{41} = V_m \cdot \text{vol}(\text{cell}) \cdot ([\text{DHFRf}] + [\text{FH2b}]) \quad (84)$$

Table 131: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V _m			0.03		<input checked="" type="checkbox"/>

7.42 Reaction FH2bdeg

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

Reaction equation



Modifier

Table 132: Properties of each modifier.

Id	Name	SBO
FH2b	dihydrofolate bound	

Product

Table 133: Properties of each product.

Id	Name	SBO
FH2f	dihydrofolate free	

Kinetic Law

Derived unit contains undeclared units

$$v_{42} = \text{vol}(\text{cell}) \cdot V_m \cdot [\text{FH2b}] \quad (86)$$

Table 134: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V_m			0.03		<input checked="" type="checkbox"/>

7.43 Reaction MTX1deg

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

Reaction equation



Reactant

Table 135: Properties of each reactant.

Id	Name	SBO
MTX1b		

Product

Table 136: Properties of each product.

Id	Name	SBO
MTX1		

Kinetic Law

Derived unit contains undeclared units

$$v_{43} = \text{vol}(\text{cell}) \cdot V_m \cdot [\text{MTX1b}] \quad (88)$$

Table 137: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V _m			0.03		<input checked="" type="checkbox"/>

7.44 Reaction MTX2deg

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

Reaction equation



Reactant

Table 138: Properties of each reactant.

Id	Name	SBO
MTX2b		

Product

Table 139: Properties of each product.

Id	Name	SBO
MTX2		

Kinetic Law

Derived unit contains undeclared units

$$v_{44} = \text{vol}(\text{cell}) \cdot V_m \cdot [\text{MTX2b}] \quad (90)$$

Table 140: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V _m			0.03		<input checked="" type="checkbox"/>

7.45 Reaction MTX3deg

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

Reaction equation



Reactant

Table 141: Properties of each reactant.

Id	Name	SBO
MTX3b		

Product

Table 142: Properties of each product.

Id	Name	SBO
MTX3		

Kinetic Law

Derived unit contains undeclared units

$$v_{45} = \text{vol}(\text{cell}) \cdot V_m \cdot [\text{MTX3b}] \quad (92)$$

Table 143: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V _m			0.03		<input checked="" type="checkbox"/>

7.46 Reaction MTX4deg

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

Reaction equation



Reactant

Table 144: Properties of each reactant.

Id	Name	SBO
MTX4b		

Product

Table 145: Properties of each product.

Id	Name	SBO
MTX4		

Kinetic Law

Derived unit contains undeclared units

$$v_{46} = \text{vol}(\text{cell}) \cdot V_m \cdot [\text{MTX4b}] \quad (94)$$

Table 146: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V _m			0.03		<input checked="" type="checkbox"/>

7.47 Reaction MTX5deg

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

Reaction equation



Reactant

Table 147: Properties of each reactant.

Id	Name	SBO
MTX5b		

Product

Table 148: Properties of each product.

Id	Name	SBO
MTX5		

Kinetic Law

Derived unit contains undeclared units

$$v_{47} = \text{vol}(\text{cell}) \cdot V_m \cdot [\text{MTX5b}] \quad (96)$$

Table 149: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vm			0.03		<input checked="" type="checkbox"/>

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 FH2f

Name dihydrofolate free

Initial concentration $0.0012 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in ten reactions (as a reactant in [DHFReductase](#), [FFH2syn](#) and as a product in [TYMS](#), [ATIC12](#), [FH2bdeg](#) and as a modifier in [MTHFR](#), [GARFT](#), [ATIC7](#), [TYMS](#), [ATIC12](#)).

$$\frac{d}{dt}\text{FH2f} = v_{11} + v_{14} + v_{42} - v_{12} - v_{13} \quad (97)$$

8.2 Species FH2b

Name dihydrofolate bound

Initial concentration $0.0024 \mu\text{mol} \cdot \text{l}^{-1}$

Involved in rule FH2b

This species takes part in three reactions (as a modifier in DHFReductase, DHFRdeg, FH2bdeg). Not these but one rule determines the species' quantity because this species is on the boundary of the reaction system.

8.3 Species DHFRf

Name dihydrofolate reductase free

Initial concentration $0.64 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in twelve reactions (as a reactant in MTX1on, MTX2on, MTX3on, MTX4on, MTX5on, DHFRdeg and as a product in MTX1off, MTX2off, MTX3off, MTX4off, MTX5off, DHFRfsyn).

$$\frac{d}{dt}\text{DHFRf} = v_{35} + v_{36} + v_{37} + v_{38} + v_{39} + v_{40} - v_{30} - v_{31} - v_{32} - v_{33} - v_{34} - v_{41} \quad (98)$$

8.4 Species DHFRtot

Name dihydrofolate reductase total

Initial concentration $0.64 \mu\text{mol} \cdot \text{l}^{-1}$

Involved in rule DHFRtot

One rule determines the species' quantity.

8.5 Species FH4

Name tetrahydrofolate

Initial concentration $0.46 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in nine reactions (as a reactant in SHMT, HCHOtoCH2FH4, HCOOHtoCHOFH4 and as a product in SHMT_r, CH2FH4toHCHO, MTR, GARFT, ATIC7, DHFReductase).

$$\frac{d}{dt}\text{FH4} = v_2 + v_4 + v_6 + v_8 + v_9 + v_{12} - v_1 - v_3 - v_7 \quad (99)$$

8.6 Species CH₂FH₄

Name 5,10-methylene-tetrahydrofolate

Initial concentration 0.26 μmol · l⁻¹

This species takes part in seven reactions (as a reactant in [SHMT_r](#), [CH₂FH₄toHCHO](#), [MTHFR](#), [MTHFD](#), [TYMS](#) and as a product in [SHMT](#), [HCHOtoCH₂FH₄](#)).

$$\frac{d}{dt}\text{CH}_2\text{FH}_4 = v_1 + v_3 - v_2 - v_4 - v_5 - v_{10} - v_{11} \quad (100)$$

8.7 Species CH₃FH₄

Name 5-methyl-tetrahydrofolate

Initial concentration 1.63 μmol · l⁻¹

This species takes part in two reactions (as a reactant in [MTR](#) and as a product in [MTHFR](#)).

$$\frac{d}{dt}\text{CH}_3\text{FH}_4 = v_5 - v_6 \quad (101)$$

8.8 Species CHO₂FH₄

Name 10-formyl-tetrahydrofolate

Initial concentration 1 μmol · l⁻¹

This species takes part in four reactions (as a reactant in [GARFT](#), [ATIC₇](#) and as a product in [HCOOHtoCHO₂FH₄](#), [MTHFD](#)).

$$\frac{d}{dt}\text{CHO}_2\text{FH}_4 = v_7 + v_{10} - v_8 - v_9 \quad (102)$$

8.9 Species FFH₂

Name 10-formyl-dihydrofolate

Initial concentration 3.32 · 10⁻⁴ μmol · l⁻¹

This species takes part in five reactions (as a reactant in [ATIC₁₂](#) and as a product in [FFH₂syn](#) and as a modifier in [GARFT](#), [ATIC₇](#), [TYMS](#)).

$$\frac{d}{dt}\text{FFH}_2 = v_{13} - v_{14} \quad (103)$$

8.10 Species HCHO

Initial concentration $0.0074 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a reactant in [HCHOtoCH2FH4](#) and as a product in [CH2FH4toHCHO](#)).

$$\frac{d}{dt}\text{HCHO} = v_4 - v_3 \quad (104)$$

8.11 Species FGAR

Initial concentration $16.49 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a reactant in [AICARsyn](#) and as a product in [GARFT](#)).

$$\frac{d}{dt}\text{FGAR} = v_8 - v_{15} \quad (105)$$

8.12 Species AICAR

Initial concentration $3.695 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in three reactions (as a reactant in [ATIC7](#), [ATIC12](#) and as a product in [AICARsyn](#)).

$$\frac{d}{dt}\text{AICAR} = v_{15} - v_9 - v_{14} \quad (106)$$

8.13 Species MTX1

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

This species takes part in twelve reactions (as a reactant in [FPGS12](#), [MTX1export](#), [MTX1on](#) and as a product in [GGH21](#), [RFC](#), [MTX1off](#), [MTX1deg](#) and as a modifier in [MTHFR](#), [GARFT](#), [ATIC7](#), [TYMS](#), [ATIC12](#)).

$$\frac{d}{dt}\text{MTX1} = v_{20} + v_{24} + v_{35} + v_{43} - v_{16} - v_{25} - v_{30} \quad (107)$$

8.14 Species MTX2

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

This species takes part in 13 reactions (as a reactant in [FPGS23](#), [GGH21](#), [MTX2export](#), [MTX2on](#) and as a product in [FPGS12](#), [GGH32](#), [MTX2off](#), [MTX2deg](#) and as a modifier in [MTHFR](#), [GARFT](#), [ATIC7](#), [TYMS](#), [ATIC12](#)).

$$\frac{d}{dt}\text{MTX2} = v_{16} + v_{21} + v_{36} + v_{44} - v_{17} - v_{20} - v_{26} - v_{31} \quad (108)$$

8.15 Species MTX3

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

This species takes part in 13 reactions (as a reactant in [FPGS34](#), [GGH32](#), [MTX3export](#), [MTX3on](#) and as a product in [FPGS23](#), [GGH43](#), [MTX3off](#), [MTX3deg](#) and as a modifier in [MTHFR](#), [GARFT](#), [ATIC7](#), [TYMS](#), [ATIC12](#)).

$$\frac{d}{dt}\text{MTX3} = v_{17} + v_{22} + v_{37} + v_{45} - v_{18} - v_{21} - v_{27} - v_{32} \quad (109)$$

8.16 Species MTX4

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

This species takes part in 13 reactions (as a reactant in [FPGS45](#), [GGH43](#), [MTX4export](#), [MTX4on](#) and as a product in [FPGS34](#), [GGH54](#), [MTX4off](#), [MTX4deg](#) and as a modifier in [MTHFR](#), [GARFT](#), [ATIC7](#), [TYMS](#), [ATIC12](#)).

$$\frac{d}{dt}\text{MTX4} = v_{18} + v_{23} + v_{38} + v_{46} - v_{19} - v_{22} - v_{28} - v_{33} \quad (110)$$

8.17 Species MTX5

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

This species takes part in eleven reactions (as a reactant in [GGH54](#), [MTX5export](#), [MTX5on](#) and as a product in [FPGS45](#), [MTX5off](#), [MTX5deg](#) and as a modifier in [MTHFR](#), [GARFT](#), [ATIC7](#), [TYMS](#), [ATIC12](#)).

$$\frac{d}{dt}\text{MTX5} = v_{19} + v_{39} + v_{47} - v_{23} - v_{29} - v_{34} \quad (111)$$

8.18 Species MTX1b

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

This species takes part in three reactions (as a reactant in [MTX1off](#), [MTX1deg](#) and as a product in [MTX1on](#)).

$$\frac{d}{dt}\text{MTX1b} = v_{30} - v_{35} - v_{43} \quad (112)$$

8.19 Species MTX2b

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

This species takes part in three reactions (as a reactant in [MTX2off](#), [MTX2deg](#) and as a product in [MTX2on](#)).

$$\frac{d}{dt}\text{MTX2b} = v_{31} - v_{36} - v_{44} \quad (113)$$

8.20 Species MTX3b

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

This species takes part in three reactions (as a reactant in [MTX3off](#), [MTX3deg](#) and as a product in [MTX3on](#)).

$$\frac{d}{dt}\text{MTX3b} = v_{32} - v_{37} - v_{45} \quad (114)$$

8.21 Species MTX4b

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

This species takes part in three reactions (as a reactant in [MTX4off](#), [MTX4deg](#) and as a product in [MTX4on](#)).

$$\frac{d}{dt}\text{MTX4b} = v_{33} - v_{38} - v_{46} \quad (115)$$

8.22 Species MTX5b

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

This species takes part in three reactions (as a reactant in [MTX5off](#), [MTX5deg](#) and as a product in [MTX5on](#)).

$$\frac{d}{dt}\text{MTX5b} = v_{34} - v_{39} - v_{47} \quad (116)$$

8.23 Species EMTX

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

This species takes part in two reactions (as a reactant in [RFC](#) and as a modifier in [DHFRfsyn](#)), which do not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{d}{dt}\text{EMTX} = 0 \quad (117)$$

8.24 Species dUMP

Initial concentration $20.76 \mu\text{mol} \cdot \text{l}^{-1}$

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

$$\frac{d}{dt}\text{dUMP} = 0 \quad (118)$$

8.25 Species GAR

Initial concentration $689.6 \mu\text{mol} \cdot \text{l}^{-1}$

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

$$\frac{d}{dt}\text{GAR} = 0 \quad (119)$$

8.26 Species serine

Initial concentration $123.3 \mu\text{mol} \cdot \text{l}^{-1}$

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

$$\frac{d}{dt}\text{serine} = 0 \quad (120)$$

8.27 Species formate

Initial concentration $500 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in one reaction (as a reactant in [HCOOHtoCHOFH4](#)), which does not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{d}{dt}\text{formate} = 0 \quad (121)$$

8.28 Species ATP

Initial concentration $2980 \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in one reaction (as a reactant in [HCOOHtoCHOFH4](#)), which does not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{d}{dt}\text{ATP} = 0 \quad (122)$$

8.29 Species glutamine

Initial concentration $7170 \mu\text{mol} \cdot \text{l}^{-1}$

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

$$\frac{d}{dt}\text{glutamine} = 0 \quad (123)$$

8.30 Species glycine

Initial concentration $1600 \mu\text{mol} \cdot \text{l}^{-1}$

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

$$\frac{d}{dt}\text{glycine} = 0 \quad (124)$$

8.31 Species NADP

Initial concentration $6.73 \mu\text{mol} \cdot \text{l}^{-1}$

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

$$\frac{d}{dt}\text{NADP} = 0 \quad (125)$$

8.32 Species NADPH

Initial concentration $294 \mu\text{mol} \cdot \text{l}^{-1}$

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

$$\frac{d}{dt}\text{NADPH} = 0 \quad (126)$$

8.33 Species homocysteine

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

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

$$\frac{d}{dt}\text{homocysteine} = 0 \quad (127)$$

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