SBML Model Report

Model name: "Hofmeyer1986_SeqFb_Proc_AA_Synthesis"

May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 3 format. This model was created by the following two authors: Lukas Endler[1] and Kieran Smallbone[2] at October tenth 2010 at 10:10 a. m. and last time modified at July fifth 2012 at 2:47 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	9
events	0	constraints	0
reactions	8	function definitions	0
global parameters	0	unit definitions	2
rules	0	initial assignments	0

Model Notes

This model is the reaction sequence SEQFB, a model pathway of a branched system with sequential feedback interactions found in bacterial amino acid synthesis. Its steady state is presented in Fig 4.

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

The model is described in:
METAMOD: software for steady-state modelling and control analysis of metabolic pathways on the BBC microcomputer.
JHS Hofmeyr and KJ van der Merwe, Comput Appl Biosci 1986 2:243-9; PubmedID: 3450367
Abstract:
METAMOD, a BBC microcomputer-based software package for steady-state modelling and control analysis of model metabolic pathways, is described, The package consists of two programs. METADEF allows the user to define the pathway in terms of reactions, rate equations and initial concentrations of metabolites. METACAL uses one of two algorithms to calculate the steady-state concentrations and fluxes. One algorithm uses the current ratio of production and consumption rates of variable metabolites to adjust iteratively their concentrations in such a way that they converge towards the steady state. The other algorithm solves the roots of the system equations by means of a quasi-Newtonian procedure. Control analysis allows the calculation of elasticity, control and response coefficients, by means of finite difference approximation. METAMOD is interactive and easy to use, and suitable for teaching and research purposes.

To cite BioModels Database, please use: Li C, Donizelli M, Rodriguez N, Dharuri H, Endler L, Chelliah V, Li L, He E, Henry A, Stefan MI, Snoep JL, Hucka M, Le Novere N, Laibe C (2010) BioModels Database: An enhanced, curated and annotated resource for published quantitative kinetic models. BMC Syst Biol., 4:92.

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`

Definition dimensionless

2.2 Unit `time`

Definition dimensionless

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 Compartment

This model contains one compartment.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
`cell`	cell	0000290	3	1	litre	☑	

3.1 Compartment `cell`

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

Name cell

SBO:0000290 physical compartment

4 Species

This model contains nine species. The boundary condition of three of these species is set to `true` so that these species' amount cannot be changed by any reaction. Section 6 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
A	A	cell	dimensionless $\cdot\, l^{-1}$	☐	☐
B	B	cell	dimensionless $\cdot\, l^{-1}$	☐	☐
C	C	cell	dimensionless $\cdot\, l^{-1}$	☐	☐
D	D	cell	dimensionless $\cdot\, l^{-1}$	☐	☐
E	E	cell	dimensionless $\cdot\, l^{-1}$	☐	☐
F	F	cell	dimensionless $\cdot\, l^{-1}$	☐	☐
X	X	cell	dimensionless $\cdot\, l^{-1}$	☑	☑
Y	Y	cell	dimensionless $\cdot\, l^{-1}$	☑	☑
Z	Z	cell	dimensionless $\cdot\, l^{-1}$	☑	☑

5 Reactions

This model contains eight 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	R1	R1	$X \overset{B}{\rightleftharpoons} A$	0000176
2	R2	R2	$A \rightleftharpoons B$	0000176
3	R3	R3	$B \overset{D}{\rightleftharpoons} C$	0000176
4	R4	R4	$C \rightleftharpoons D$	0000176
5	R5	R5	$D \rightleftharpoons Y$	0000176
6	R6	R6	$B \overset{F}{\rightleftharpoons} E$	0000176
7	R7	R7	$E \rightleftharpoons F$	0000176
8	R8	R8	$F \rightleftharpoons Z$	0000176

5.1 Reaction R1

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

Name R1

SBO:0000176 biochemical reaction

Reaction equation

$$\mathrm{X} \overset{\mathrm{B}}{\rightleftharpoons} \mathrm{A} \tag{1}$$

Reactant

Table 5: Properties of each reactant.

Id	Name	SBO
X	X	

Modifier

Table 6: Properties of each modifier.

Id	Name	SBO
B	B	0000206

Product

Table 7: Properties of each product.

Id	Name	SBO
A	A	

Kinetic Law

SBO:0000430 enzymatic rate law for modulated unireactant enzymes

Derived unit contains undeclared units

$$v_1 = \mathrm{vol}\,(\mathrm{cell}) \cdot \frac{10 \cdot [\mathrm{X}] - [\mathrm{A}]}{1 + [\mathrm{X}] + [\mathrm{A}] + [\mathrm{B}]^2} \tag{2}$$

5.2 Reaction R2

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

Name R2

SBO:0000176 biochemical reaction

Reaction equation

$$\mathrm{A} \rightleftharpoons \mathrm{B} \tag{3}$$

Reactant

Table 8: Properties of each reactant.

Id	Name	SBO
A	A	

Product

Table 9: Properties of each product.

Id	Name	SBO
B	B	

Kinetic Law

SBO:0000326 enzymatic rate law for non-modulated unireactant enzymes

Derived unit contains undeclared units

$$v_2 = \mathrm{vol}\,(\mathrm{cell}) \cdot \frac{2 \cdot [\mathrm{A}] - [\mathrm{B}]}{1 + [\mathrm{A}] + [\mathrm{B}]} \tag{4}$$

5.3 Reaction R3

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

Name R3

SBO:0000176 biochemical reaction

Reaction equation

$$\mathrm{B} \overset{\mathrm{D}}{\rightleftharpoons} \mathrm{C} \tag{5}$$

Reactant

Table 10: Properties of each reactant.

Id	Name	SBO
B	B	

Modifier

Table 11: Properties of each modifier.

Id	Name	SBO
D	D	0000206

Product

Table 12: Properties of each product.

Id	Name	SBO
C	C	

Kinetic Law

SBO:0000430 enzymatic rate law for modulated unireactant enzymes

Derived unit contains undeclared units

$$v_3 = \mathrm{vol}\,(\mathrm{cell}) \cdot \frac{[\mathrm{B}] - [\mathrm{C}]}{1 + [\mathrm{B}] + [\mathrm{C}] + [\mathrm{D}]^2} \tag{6}$$

5.4 Reaction R4

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

Name R4

SBO:0000176 biochemical reaction

Reaction equation

$$\mathrm{C} \rightleftharpoons \mathrm{D} \tag{7}$$

Reactant

Table 13: Properties of each reactant.

Id	Name	SBO
C	C	

Product

Table 14: Properties of each product.

Id	Name	SBO
D	D	

Kinetic Law

SBO:0000326 enzymatic rate law for non-modulated unireactant enzymes

Derived unit contains undeclared units

$$v_4 = \mathrm{vol}\,(\mathrm{cell}) \cdot \frac{5 \cdot [\mathrm{C}] - [\mathrm{D}]}{1 + [\mathrm{C}] + [\mathrm{D}]} \tag{8}$$

5.5 Reaction R5

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

Name R5

SBO:0000176 biochemical reaction

Reaction equation

$$\mathrm{D} \rightleftharpoons \mathrm{Y} \tag{9}$$

Reactant

Table 15: Properties of each reactant.

Id	Name	SBO
D	D	

Product

Table 16: Properties of each product.

Id	Name	SBO
Y	Y	

Kinetic Law

SBO:0000326 enzymatic rate law for non-modulated unireactant enzymes

Derived unit contains undeclared units

$$v_5 = \mathrm{vol}\,(\mathrm{cell}) \cdot \frac{10 \cdot [\mathrm{D}] - [\mathrm{Y}]}{1 + [\mathrm{D}] + [\mathrm{Y}]} \tag{10}$$

5.6 Reaction R6

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

Name R6

SBO:0000176 biochemical reaction

Reaction equation

$$\mathrm{B} \overset{\mathrm{F}}{\rightleftharpoons} \mathrm{E} \tag{11}$$

Reactant

Table 17: Properties of each reactant.

Id	Name	SBO
B	B	

Modifier

Table 18: Properties of each modifier.

Id	Name	SBO
F	F	0000206

Product

Table 19: Properties of each product.

Id	Name	SBO
E	E	

Kinetic Law

SBO:0000430 enzymatic rate law for modulated unireactant enzymes

Derived unit contains undeclared units

$$v_6 = \mathrm{vol}\,(\mathrm{cell}) \cdot \frac{[\mathrm{B}] - [\mathrm{E}]}{1 + [\mathrm{B}] + [\mathrm{E}] + [\mathrm{F}]^2} \tag{12}$$

5.7 Reaction R7

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

Name R7

SBO:0000176 biochemical reaction

Reaction equation

$$\mathrm{E} \rightleftharpoons \mathrm{F} \tag{13}$$

Reactant

Table 20: Properties of each reactant.

Id	Name	SBO
E	E	

Product

Table 21: Properties of each product.

Id	Name	SBO
F	F	

Kinetic Law

SBO:0000326 enzymatic rate law for non-modulated unireactant enzymes

Derived unit contains undeclared units

$$v_7 = \mathrm{vol}\,(\mathrm{cell}) \cdot \frac{5 \cdot [\mathrm{E}] - [\mathrm{F}]}{1 + [\mathrm{E}] + [\mathrm{F}]} \tag{14}$$

5.8 Reaction R8

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

Name R8

SBO:0000176 biochemical reaction

Reaction equation

$$\mathrm{F} \rightleftharpoons \mathrm{Z} \tag{15}$$

Reactant

Table 22: Properties of each reactant.

Id	Name	SBO
F	F	

Product

Table 23: Properties of each product.

Id	Name	SBO
Z	Z	

Kinetic Law

SBO:0000326 enzymatic rate law for non-modulated unireactant enzymes

Derived unit contains undeclared units

$$v_8 = \mathrm{vol}\,(\mathrm{cell}) \cdot \frac{10 \cdot [\mathrm{F}] - [\mathrm{Z}]}{1 + [\mathrm{F}] + [\mathrm{Z}]} \tag{16}$$

6 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.

6.1 Species A

Name A

SBO:0000247 simple chemical

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

This species takes part in two reactions (as a reactant in R2 and as a product in R1).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{A} = v_1 - v_2 \tag{17}$$

6.2 Species B

Name B

SBO:0000247 simple chemical

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

This species takes part in four reactions (as a reactant in R3, R6 and as a product in R2 and as a modifier in R1).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{B} = v_2 - v_3 - v_6 \tag{18}$$

6.3 Species C

Name C

SBO:0000247 simple chemical

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

This species takes part in two reactions (as a reactant in R4 and as a product in R3).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C} = v_3 - v_4 \tag{19}$$

6.4 Species D

Name D

SBO:0000247 simple chemical

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

This species takes part in three reactions (as a reactant in R5 and as a product in R4 and as a modifier in R3).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{D} = v_4 - v_5 \tag{20}$$

6.5 Species E

Name E

SBO:0000247 simple chemical

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

This species takes part in two reactions (as a reactant in R7 and as a product in R6).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{E} = v_6 - v_7 \tag{21}$$

6.6 Species F

Name F

SBO:0000247 simple chemical

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

This species takes part in three reactions (as a reactant in R8 and as a product in R7 and as a modifier in R6).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{F} = v_7 - v_8 \tag{22}$$

6.7 Species X

Name X

SBO:0000247 simple chemical

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

This species takes part in one reaction (as a reactant in R1), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{X} = 0 \tag{23}$$

6.8 Species Y

Name Y

SBO:0000247 simple chemical

Initial concentration $2\ \text{dimensionless} \cdot \text{l}^{-1}$

This species takes part in one reaction (as a product in R5), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Y} = 0 \tag{24}$$

6.9 Species Z

Name Z

SBO:0000247 simple chemical

Initial concentration $1\ \text{dimensionless} \cdot \text{l}^{-1}$

This species takes part in one reaction (as a product in R8), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Z} = 0 \tag{25}$$

A Glossary of Systems Biology Ontology Terms

SBO:0000176 biochemical reaction: An event involving one or more chemical entities that modifies the electrochemical structure of at least one of the participants.

SBO:0000206 competitive inhibitor: Substance that decreases the probability of a chemical reaction, without itself being consumed or transformed by the reaction, by stericaly hindering the interaction between reactants

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

SBO:0000290 physical compartment: Specific location of space, that can be bounded or not. A physical compartment can have 1, 2 or 3 dimensions

SBO:0000326 enzymatic rate law for non-modulated unireactant enzymes: Kinetics of enzymes that react only with one substance, their substrate, and are not modulated by other compounds

SBO:0000430 enzymatic rate law for modulated unireactant enzymes: Kinetics of enzymes that react with one substance, and whose activity may be positively or negatively modulated

SBML2LaTeX was developed by Andreas Dräger[a], Hannes Planatscher[a], Dieudonné M Wouamba[a], Adrian Schröder[a], Michael Hucka[b], Lukas Endler[c], Martin Golebiewski[d] and Andreas Zell[a]. Please see http://www.ra.cs.uni-tuebingen.de/software/SBML2LaTeX for more information.

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