SBML Model Report

Model name: "Klipp2002-_MetabolicOptimization_linearPathway(n=2)"

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1 General Overview

This is a document in SBML Level 2 Version 1 format. This model was created by the following three authors: Nicolas Le Novre[1], Enuo He[2] and Nick Juty[3] at March 26th 2007 at 9:35 a. m. and last time modified at February 25th 2015 at 12:24 a. 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	6
events	1	constraints	0
reactions	2	function definitions	0
global parameters	0	unit definitions	0
rules	1	initial assignments	0

Model Notes

Klipp2002_MetabolicOptimization_linearPathway(n=2)

The model describes time dependent gene expression as a means to enable cells to adapt metabolic activity optimally based on environmental conditions. It uses a simple unbranched

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pathway and a constraint of fixed total enzyme. It calculates enzyme profiles at different times which optimise a performance function, and compares them to experimental data. The initial model is cell-type agnostic, while the experimeental data is from yeast.

This model is described in the article:Prediction of temporal gene expression. Metabolic opimization by re-distribution of enzyme activities.Klipp E, Heinrich R, Holzhtter HG.Eur. J. Biochem. 2002 Nov; 269(22): 5406-5413

Abstract:

A computational approach is used to analyse temporal gene expression in the context of metabolic regulation. It is based on the assumption that cells developed optimal adaptation strategies to changing environmental conditions. Time- dependent enzyme profiles are calculated which optimize the function of a metabolic pathway under the constraint of limited total enzyme amount. For linear model pathways it is shown that wave-like enzyme profiles are optimal for a rapid substrate turnover. For the central metabolism of yeast cells enzyme profiles are calculated which ensure long-term homeostasis of key metabolites under conditions of a diauxic shift. These enzyme profiles are in close correlation with observed gene expression data. Our results demonstrate that optimality principles help to rationalize observed gene expression profiles.

This model is from the paper *Prediction of temporal gene expression metabolic optimization by re-distribution of enzyme activities.* The model describes optimal enzyme profiles and metabolite time courses for a simple linear metabolic pathway (n=2). Figure 1 was reproduced using roadRunner. The values of k1 and k2 were not explicitly stated in the publication, but calculations were performed for equal catalytic efficiencies of the enzymes (ki=k), hence the curator assigned k1=k2=1. Also enzyme concentrations are given in units of Etot; times are given in units of 1/(k*Etot) in the papaer, for simplicity , we use defalut units of the SBML to present the concentration and time.

This model is hosted on BioModels Database and identifiedby: MODEL4931762955 .

To cite BioModels Database, please use: BioModels Database: An enhanced, curated and annotated resourcefor published quantitative kinetic models .

2 Unit Definitions

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

2.1 Unit `substance`

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

Definition mol

2.2 Unit volume

Notes Litre is the predefined SBML unit for volume.

Definition l

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_0	cell		3	1	litre	☑	

3.1 Compartment compartment_0

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

Name cell

4 Species

This model contains six species. 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
species_0	S	compartment_0	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☐
species_1	X1	compartment_0	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☐
species_2	E1	compartment_0	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☐
species_3	E2	compartment_0	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☐
species_4	P	compartment_0	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☐
species_5	Etot	compartment_0	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☑	☐

5 Rule

This is an overview of one rule.

5.1 Rule species_3

Rule species_3 is an assignment rule for species species_3:

$$\text{species\_3} = [\text{species\_5}] - [\text{species\_2}] \tag{1}$$

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

6 Event

This is an overview of one event. Each event is initiated whenever its trigger condition switches from false to true. A delay function postpones the effects of an event to a later time point. At the time of execution, an event can assign values to species, parameters or compartments if these are not set to constant.

6.1 Event event_0000002

Name single switch

Notes During the initial phase, t smaller than T1 (T1=1), the whole amount of protein is allocated to the first reaction(E1=Etot, E2=0). At the beginning of the second phase the concentration E2 undergoes an abrupt switch from zero to a finite vaule whereas the concentration E1 is descreased by the same extent.

Trigger condition

$$\text{time} > 1 \tag{2}$$

Assignment

$$\text{species\_2} = 0.4 \tag{3}$$

7 Reactions

This model contains two 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	`reaction_0`	S->X1	$\text{species\_0} \xrightarrow{\text{species\_2}} \text{species\_1}$	
2	`reaction_1`	X1->P	$\text{species\_1} \xrightarrow{\text{species\_3}} \text{species\_4}$	

7.1 Reaction reaction_0

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

Name S->X1

Reaction equation

$$\text{species\_0} \xrightarrow{\text{species\_2}} \text{species\_1} \tag{4}$$

Reactant

Table 5: Properties of each reactant.

Id	Name	SBO
species_0	S	

Modifier

Table 6: Properties of each modifier.

Id	Name	SBO
species_2	E1	

Product

Table 7: Properties of each product.

Id	Name	SBO
species_1	X1	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \text{vol}(\text{compartment\_0}) \cdot [\text{species\_0}] \cdot [\text{species\_2}] \cdot \text{k1} \tag{5}$$

Table 8: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1			1.0		☑

7.2 Reaction reaction_1

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

Name X1->P

Reaction equation

$$\text{species\_1} \xrightarrow{\text{species\_3}} \text{species\_4} \tag{6}$$

Reactant

Table 9: Properties of each reactant.

Id	Name	SBO
species_1	X1	

Modifier

Table 10: Properties of each modifier.

Id	Name	SBO
species_3	E2	

Product

Table 11: Properties of each product.

Id	Name	SBO
species_4	P	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \text{vol}\left(\text{compartment\_0}\right) \cdot \text{k2} \cdot [\text{species\_1}] \cdot [\text{species\_3}] \tag{7}$$

Table 12: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k2			1.0		☑

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 `species_0`

Name S

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

This species takes part in one reaction (as a reactant in `reaction_0`).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_0} = -\ v_1 \tag{8}$$

8.2 Species `species_1`

Name X1

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

This species takes part in two reactions (as a reactant in `reaction_1` and as a product in `reaction_0`).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_1} = v_1 - v_2 \tag{9}$$

8.3 Species `species_2`

Name E1

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

Involved in event `event_0000002`

This species takes part in one reaction (as a modifier in `reaction_0`).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_2} = 0 \tag{10}$$

Furthermore, one event influences this species' rate of change.

8.4 Species species_3

Name E2

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

Involved in rule species_3

This species takes part in one reaction (as a modifier in reaction_1) and is also involved in one rule which determines this species' quantity.

8.5 Species species_4

Name P

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

This species takes part in one reaction (as a product in reaction_1).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_4} = v_2 \tag{11}$$

8.6 Species species_5

Name Etot

Notes Etot=E1+E2 is constant.

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_5} = 0 \tag{12}$$

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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