SBML Model Report

Model name: “Smallbone2013 - Metabolic Control Analysis - Example 2”

May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by the following two authors: Vijayalakshmi Chelliah[1] and Kieran Smallbone[2] at May first 2013 at noon. and last time modified at April eighth 2016 at 5:28 p. m. Table 1 provides 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	5	function definitions	0
global parameters	0	unit definitions	3
rules	0	initial assignments	0

Model Notes

Smallbone2013 - Metabolic Control Analysis - Example 2

Metabolic control analysis (MCA) is a biochemical formalism, defining how variables, such as fluxes and concentrations, depend on network parameters. In this paper, owing to its limitations,

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

it is shown with three example models (MODEL1305030000-2) that the algorithm with slight modification can be applied to all models.

This model is described in the article:Metabolic Control Analysis: Rereading RederKieran SmallboneQuantitative Methods; Tue, 28 May 2013.

Abstract:

Metabolic control analysis is a biochemical formalism defined by Kacser and Burns in 1973, and given firm mathematical basis by Reder in 1988. The algorithm defined by Reder for calculating the control matrices is still used by software programs today, but is only valid for some biochemical models. We show that, with slight modification, the algorithm may be applied to all models.

This model is hosted on BioModels Database and identifiedby: MODEL1305030001 .

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 of which two 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`

Definition dimensionless

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	dimensionless	☑	

3.1 Compartment `cell`

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

Name cell

SBO:0000290 physical compartment

4 Species

This model contains nine species. The boundary condition of six 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
x1	x1	cell	dimensionless · dimensionless^{-1}	⊟	⊟
x2	x2	cell	dimensionless · dimensionless^{-1}	⊟	⊟
x3	x3	cell	dimensionless · dimensionless^{-1}	⊟	⊟
y1	y1	cell	dimensionless · dimensionless^{-1}	☑	☑
y2	y2	cell	dimensionless · dimensionless^{-1}	☑	☑
y3	y3	cell	dimensionless · dimensionless^{-1}	☑	☑
y4	y4	cell	dimensionless · dimensionless^{-1}	☑	☑
y5	y5	cell	dimensionless · dimensionless^{-1}	☑	☑
y6	y6	cell	dimensionless · dimensionless^{-1}	☑	☑

5 Reactions

This model contains five 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	v1	v1	$\mathrm{y1} + \mathrm{x2} \xrightleftharpoons{\mathrm{y1,\ x2,\ x1,\ x3}} \mathrm{x1} + \mathrm{x3}$	0000176
2	v2	v2	$\mathrm{y4} + \mathrm{x3} \xrightleftharpoons{\mathrm{y4,\ x3,\ y5,\ x2}} \mathrm{y5} + \mathrm{x2}$	0000176
3	v3	v3	$\mathrm{x1} \xrightleftharpoons{\mathrm{x1,\ y2}} \mathrm{y2}$	0000176
4	v4	v4	$\mathrm{x1} \xrightleftharpoons{\mathrm{x1,\ y3}} \mathrm{y3}$	0000176
5	v5	v5	$\mathrm{x3} \xrightleftharpoons{\mathrm{x3}} \mathrm{y6}$	0000176

5.1 Reaction v1

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

Name v1

SBO:0000176 biochemical reaction

Reaction equation

$$\mathrm{y1} + \mathrm{x2} \xrightleftharpoons{\mathrm{y1},\ \mathrm{x2},\ \mathrm{x1},\ \mathrm{x3}} \mathrm{x1} + \mathrm{x3} \tag{1}$$

Reactants

Table 5: Properties of each reactant.

Id	Name	SBO
y1	y1	
x2	x2	

Modifiers

Table 6: Properties of each modifier.

Id	Name	SBO
y1	y1	
x2	x2	
x1	x1	
x3	x3	

Products

Table 7: Properties of each product.

Id	Name	SBO
x1	x1	
x3	x3	

Kinetic Law

SBO:0000430 enzymatic rate law for modulated unireactant enzymes

Derived unit contains undeclared units

$$v_1 = \frac{\mathrm{e1} \cdot (\mathrm{p1} \cdot [\mathrm{y1}] \cdot [\mathrm{x2}] - [\mathrm{x1}] \cdot [\mathrm{x3}])}{1 + [\mathrm{y1}] + [\mathrm{x2}] + [\mathrm{x1}] + [\mathrm{x3}] + [\mathrm{y1}] \cdot [\mathrm{x2}] + [\mathrm{x1}] \cdot [\mathrm{x3}]} \tag{2}$$

Table 8: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
e1			1.0	dimensionless	☑
p1			10.0	dimensionless	☑

5.2 Reaction v2

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

Name v2

SBO:0000176 biochemical reaction

Reaction equation

$$\mathrm{y4} + \mathrm{x3} \overset{\mathrm{y4,\ x3,\ y5,\ x2}}{\rightleftharpoons} \mathrm{y5} + \mathrm{x2} \tag{3}$$

Reactants

Table 9: Properties of each reactant.

Id	Name	SBO
y4	y4	
x3	x3	

Modifiers

Table 10: Properties of each modifier.

Id	Name	SBO
y4	y4	
x3	x3	
y5	y5	
x2	x2	

Products

Table 11: Properties of each product.

Id	Name	SBO
y5	y5	
x2	x2	

Kinetic Law

SBO:0000430 enzymatic rate law for modulated unireactant enzymes

Derived unit contains undeclared units

$$v_2 = \frac{\mathrm{e2} \cdot (\mathrm{p2} \cdot [\mathrm{y4}] \cdot [\mathrm{x3}] - [\mathrm{y5}] \cdot [\mathrm{x2}])}{1 + [\mathrm{x3}] + [\mathrm{x2}] + [\mathrm{y4}] + [\mathrm{y5}] + [\mathrm{x3}] \cdot [\mathrm{y4}] + [\mathrm{x2}] \cdot [\mathrm{y5}]} \tag{4}$$

Table 12: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
e2			1.0	dimensionless	☑
p2			10.0	dimensionless	☑

5.3 Reaction v3

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

Name v3

SBO:0000176 biochemical reaction

Reaction equation

$$\mathrm{x1} \overset{\mathrm{x1,\ y2}}{\rightleftharpoons} \mathrm{y2} \tag{5}$$

Reactant

Table 13: Properties of each reactant.

Id	Name	SBO
x1	x1	

Modifiers

Table 14: Properties of each modifier.

Id	Name	SBO
x1	x1	
y2	y2	

Product

Table 15: Properties of each product.

Id	Name	SBO
y2	y2	

Kinetic Law

SBO:0000430 enzymatic rate law for modulated unireactant enzymes

Derived unit contains undeclared units

$$v_3 = \frac{\mathrm{e3} \cdot (\mathrm{p3} \cdot [\mathrm{x1}] - [\mathrm{y2}])}{1 + [\mathrm{x1}] + [\mathrm{y2}]} \tag{6}$$

Table 16: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
e3			1.0	dimensionless	☑
p3			50.0	dimensionless	☑

5.4 Reaction v4

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

Name v4

SBO:0000176 biochemical reaction

Reaction equation

$$\mathrm{x1} \overset{\mathrm{x1,\ y3}}{\rightleftharpoons} \mathrm{y3} \tag{7}$$

Reactant

Table 17: Properties of each reactant.

Id	Name	SBO
x1	x1	

Modifiers

Table 18: Properties of each modifier.

Id	Name	SBO
x1	x1	
y3	y3	

Product

Table 19: Properties of each product.

Id	Name	SBO
y3	y3	

Kinetic Law

SBO:0000430 enzymatic rate law for modulated unireactant enzymes

Derived unit contains undeclared units

$$v_4 = \frac{\mathrm{e4} \cdot (\mathrm{p4} \cdot [\mathrm{x1}] - [\mathrm{y3}])}{1 + [\mathrm{x1}] + [\mathrm{y3}]} \tag{8}$$

Table 20: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
e4			1.0	dimensionless	☑
p4			10.0	dimensionless	☑

5.5 Reaction v5

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

Name v5

SBO:0000176 biochemical reaction

Reaction equation

$$\mathrm{x3} \overset{\mathrm{x3}}{\rightleftharpoons} \mathrm{y6} \tag{9}$$

Reactant

Table 21: Properties of each reactant.

Id	Name	SBO
x3	x3	

Modifier

Table 22: Properties of each modifier.

Id	Name	SBO
x3	x3	

Product

Table 23: Properties of each product.

Id	Name	SBO
y6	y6	

Kinetic Law

SBO:0000430 enzymatic rate law for modulated unireactant enzymes

Derived unit $\mathrm{dimensionless}^{-1}$

$$v_5 = \mathrm{e5} \cdot \mathrm{p5} \cdot [\mathrm{x3}] \tag{10}$$

Table 24: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
e5			1.0	dimensionless	☑
p5			0.0	dimensionless	☑

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 x1

Name x1

SBO:0000247 simple chemical

Initial concentration 0.05625738310526 dimensionless $\cdot$ dimensionless^{-1}

This species takes part in six reactions (as a reactant in v3, v4 and as a product in v1 and as a modifier in v1, v3, v4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{x1} = v_1 - v_3 - v_4 \tag{11}$$

6.2 Species x2

Name x2

SBO:0000247 simple chemical

Initial concentration 0.76876151899652 dimensionless $\cdot$ dimensionless^{-1}

This species takes part in four reactions (as a reactant in v1 and as a product in v2 and as a modifier in v1, v2).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{x2} = v_2 - v_1 \tag{12}$$

6.3 Species x3

Name x3

SBO:0000247 simple chemical

Initial concentration 4.23123848100348 dimensionless $\cdot$ dimensionless^{-1}

This species takes part in six reactions (as a reactant in v2, v5 and as a product in v1 and as a modifier in v1, v2, v5).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{x3} = v_1 - v_2 - v_5 \tag{13}$$

6.4 Species y1

Name y1

SBO:0000247 simple chemical

Initial concentration 10 dimensionless · dimensionless^{-1}

This species takes part in two reactions (as a reactant in v1 and as a modifier in v1), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{y1} = 0 \tag{14}$$

6.5 Species y2

Name y2

SBO:0000247 simple chemical

Initial concentration 0 dimensionless · dimensionless^{-1}

This species takes part in two reactions (as a product in v3 and as a modifier in v3), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{y2} = 0 \tag{15}$$

6.6 Species y3

Name y3

SBO:0000247 simple chemical

Initial concentration 0 dimensionless · dimensionless^{-1}

This species takes part in two reactions (as a product in v4 and as a modifier in v4), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{y3} = 0 \tag{16}$$

6.7 Species y4

Name y4

SBO:0000247 simple chemical

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

This species takes part in two reactions (as a reactant in v2 and as a modifier in v2), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{y4} = 0 \tag{17}$$

6.8 Species y5

Name y5

SBO:0000247 simple chemical

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

This species takes part in two reactions (as a product in v2 and as a modifier in v2), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{y5} = 0 \tag{18}$$

6.9 Species y6

Name y6

SBO:0000247 simple chemical

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

This species takes part in one reaction (as a product in v5), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{y6} = 0 \tag{19}$$

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: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: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