SBML Model Report

Model name: "Shen-Orr2002_Single_Input_Module"

May 5, 2016

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by Kieran Smallbone[1] at February eighth 2011 at no o' clock in the morning. and last time modified at March 31st 2014 at 12:16 a. 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	4
events	2	constraints	0
reactions	6	function definitions	1
global parameters	1	unit definitions	3
rules	1	initial assignments	0

Model Notes

This is the single input module, SIM, described in the article:
Network motifs in the transcriptional regulation network of Escherichia coli
Shai S. Shen-Orr, Ron Milo, Shmoolik Mangan, Uri Alon, *Nat Genet* 2002 31:64-68; PMID:11967538; DOI:10.1038/ng881;

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Abstract:
Little is known about the design principles of transcriptional regulation networks that control gene expression in cells. Recent advances in data collection and analysis, however, are generating unprecedented amounts of information about gene regulation networks. To understand these complex wiring diagrams, we sought to break down such networks into basic building blocks. We generalize the notion of motifs, widely used for sequence analysis, to the level of networks. We define 'network motifs' as patterns of interconnections that recur in many different parts of a network at frequencies much higher than those found in randomized networks. We applied new algorithms for systematically detecting network motifs to one of the best-characterized regulation networks, that of direct transcriptional interactions in Escherichia coli. We find that much of the network is composed of repeated appearances of three highly significant motifs. Each network motif has a specific function in determining gene expression, such as generating temporal expression programs and governing the responses to fluctuating external signals. The motif structure also allows an easily interpretable view of the entire known transcriptional network of the organism. This approach may help define the basic computational elements of other biological networks.

This model reproduces the SIM timecourse presented in Figure 2b. All species and parameters in the model are dimensionless.

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 four species. The boundary condition of one of these species is set to `true` so that this species' amount cannot be changed by any reaction. Section 10 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
`X`		`cell`	dimensionless $\cdot$ dimensionless^{-1}	⊟	☑
`Z1`		`cell`	dimensionless $\cdot$ dimensionless^{-1}	⊟	⊟
`Z2`		`cell`	dimensionless $\cdot$ dimensionless^{-1}	⊟	⊟
`Z3`		`cell`	dimensionless $\cdot$ dimensionless^{-1}	⊟	⊟

5 Parameter

This model contains one global parameter.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
FX			0.0	dimensionless	⊟

6 Function definition

This is an overview of one function definition.

6.1 Function definition F

Arguments [X], T

Mathematical Expression

$$\begin{cases} 1 & \text{if } [\mathrm{X}] \geq \mathrm{T} \\ 0 & \text{otherwise} \end{cases} \tag{1}$$

7 Rule

This is an overview of one rule.

7.1 Rule X

Rule X is a rate rule for species X:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{X} = \mathrm{FX} - [\mathrm{X}] \tag{2}$$

Derived unit dimensionless

8 Events

This is an overview of two events. 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.

8.1 Event e1

Trigger condition

$$\text{time} \geq 1 \tag{3}$$

Assignment

$$\text{FX} = 1 \tag{4}$$

8.2 Event e2

Trigger condition

$$\text{time} \geq 6 \tag{5}$$

Assignment

$$\text{FX} = 0 \tag{6}$$

9 Reactions

This model contains six 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

№	Id	Name	Reaction Equation	SBO
1	r1		$\emptyset \overset{X}{\rightleftharpoons} Z1$	0000205
2	r2		$Z1 \rightleftharpoons \emptyset$	0000179
3	r3		$\emptyset \overset{X}{\rightleftharpoons} Z2$	0000205
4	r4		$Z2 \rightleftharpoons \emptyset$	0000179
5	r5		$\emptyset \overset{X}{\rightleftharpoons} Z3$	0000205
6	r6		$Z3 \rightleftharpoons \emptyset$	0000179

9.1 Reaction r1

This is a reversible reaction of no reactant forming one product influenced by one modifier.

SBO:0000205 composite biochemical process

Reaction equation

$$\emptyset \overset{\mathrm{X}}{\rightleftharpoons} \mathrm{Z1} \tag{7}$$

Modifier

Table 6: Properties of each modifier.

Id	Name	SBO
X		

Product

Table 7: Properties of each product.

Id	Name	SBO
Z1		

Kinetic Law

Derived unit not available

$$v_1 = \mathrm{F}([\mathrm{X}], \mathrm{T1}) \tag{8}$$

$$\mathrm{F}([\mathrm{X}], \mathrm{T}) = \begin{cases} 1 & \text{if } [\mathrm{X}] \geq \mathrm{T} \\ 0 & \text{otherwise} \end{cases} \tag{9}$$

Table 8: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
T1			0.1	dimensionless	☑

9.2 Reaction r2

This is a reversible reaction of one reactant forming no product.

SBO:0000179 degradation

Reaction equation

$$\mathrm{Z1} \rightleftharpoons \emptyset \tag{10}$$

Reactant

Table 9: Properties of each reactant.

Id	Name	SBO
Z1		

Kinetic Law

Derived unit dimensionless^{-1}

$$v_2 = \mathrm{a} \cdot [\mathrm{Z1}] \tag{11}$$

Table 10: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
a			1.0	dimensionless	☑

9.3 Reaction r3

This is a reversible reaction of no reactant forming one product influenced by one modifier.

SBO:0000205 composite biochemical process

Reaction equation

$$\emptyset \overset{\mathrm{X}}{\rightleftharpoons} \mathrm{Z2} \tag{12}$$

Modifier

Table 11: Properties of each modifier.

Id	Name	SBO
X		

Product

Table 12: Properties of each product.

Id	Name	SBO
Z2		

Kinetic Law

Derived unit not available

$$v_3 = \mathrm{F}([\mathrm{X}], \mathrm{T2}) \tag{13}$$

$$\mathrm{F}([\mathrm{X}], \mathrm{T}) = \begin{cases} 1 & \text{if } [\mathrm{X}] \geq \mathrm{T} \\ 0 & \text{otherwise} \end{cases} \tag{14}$$

Table 13: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
T2			0.5	dimensionless	☑

9.4 Reaction r4

This is a reversible reaction of one reactant forming no product.

SBO:0000179 degradation

Reaction equation

$$\mathrm{Z2} \rightleftharpoons \emptyset \tag{15}$$

Reactant

Table 14: Properties of each reactant.

Id	Name	SBO
Z2		

Kinetic Law

Derived unit dimensionless^{-1}

$$v_4 = \mathrm{a} \cdot [\mathrm{Z2}] \tag{16}$$

Table 15: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
a			1.0	dimensionless	☑

9.5 Reaction r5

This is a reversible reaction of no reactant forming one product influenced by one modifier.

SBO:0000205 composite biochemical process

Reaction equation

$$\emptyset \overset{\mathrm{X}}{\rightleftharpoons} \mathrm{Z3} \tag{17}$$

Modifier

Table 16: Properties of each modifier.

Id	Name	SBO
X		

Product

Table 17: Properties of each product.

Id	Name	SBO
Z3		

Kinetic Law

Derived unit not available

$$v_5 = \mathrm{F}([\mathrm{X}], \mathrm{T3}) \tag{18}$$

$$\mathrm{F}([\mathrm{X}], \mathrm{T}) = \begin{cases} 1 & \text{if } [\mathrm{X}] \geq \mathrm{T} \\ 0 & \text{otherwise} \end{cases} \tag{19}$$

Table 18: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
T3			0.8	dimensionless	☑

9.6 Reaction r6

This is a reversible reaction of one reactant forming no product.

SBO:0000179 degradation

Reaction equation

$$\mathrm{Z3} \rightleftharpoons \emptyset \tag{20}$$

Reactant

Table 19: Properties of each reactant.

Id	Name	SBO
Z3		

Kinetic Law

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

$$v_6 = \mathrm{a} \cdot [\mathrm{Z3}] \tag{21}$$

Table 20: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
a			1.0	dimensionless	☑

10 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.

10.1 Species X

SBO:0000252 polypeptide chain

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

Involved in rule X

This species takes part in three reactions (as a modifier in r1, r3, r5). Not these but one rule determines the species' quantity because this species is on the boundary of the reaction system.

10.2 Species Z1

SBO:0000252 polypeptide chain

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

This species takes part in two reactions (as a reactant in r2 and as a product in r1).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Z1} = v_1 - v_2 \tag{22}$$

10.3 Species Z2

SBO:0000252 polypeptide chain

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

This species takes part in two reactions (as a reactant in r4 and as a product in r3).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Z2} = v_3 - v_4 \tag{23}$$

10.4 Species Z3

SBO:0000252 polypeptide chain

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

This species takes part in two reactions (as a reactant in r6 and as a product in r5).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Z3} = v_5 - v_6 \tag{24}$$

A Glossary of Systems Biology Ontology Terms

SBO:0000179 **degradation:** Complete disappearance of a physical entity

SBO:0000205 **composite biochemical process:** Process that involves the participation of chemical or biological entities and is composed of several elementary steps or reactions.

SBO:0000252 **polypeptide chain:** Naturally occurring macromolecule formed by the repetition of amino-acid residues linked by peptidic bonds. A polypeptide chain is synthesized by the ribosome. CHEBI:1654

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

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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