SBML Model Report

Model name: “Liebal2012 - B.subtilis transcription inhibition model”

May 5, 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 Ulf Liebal[2] at June sixth 2013 at 7:36 p. m. and last time modified at May 30th 2014 at 4:05 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	1
species types	0	species	4
events	0	constraints	0
reactions	3	function definitions	0
global parameters	6	unit definitions	0
rules	0	initial assignments	0

Model Notes

Liebal2012 - B.subtilis transcription inhibition model

An important transcription factor of B.subsilis is sigma ^{B} . Liebal et al. (2012) have performed experiments in B.subtilis wild type and mutant straits to test and validate a mathematical model of the dynamics of sigma ^{B} activity. The following three models are constructed

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and their ability to fit the experimental data were tested. 1) Transcription inhibition model (MODEL1212180000), 2) sigma ^{B} proteolysis model (MODEL1302080000) and 3) Post-transcriptional instability model (MODEL1302080001). This model corresponds to the Transcription inhibition model (MODEL1212180000).

This model is described in the article:Proteolysis of beta-galactosidase following SigmaB activation in Bacillus subtilis.Liebal UW, Sappa PK, Millat T, Steil L, Homuth G, Vlker U, Wolkenhauer O.2012 Jun;8(6):1806-14.

Abstract:

In Bacillus subtilis the (B) mediated general stress response provides protection against various environmental and energy related stress conditions. To better understand the general stress response, we need to explore the mechanism by which the components interact. Here, we performed experiments in B. subtilis wild type and mutant strains to test and validate a mathematical model of the dynamics of (B) activity. In the mutant strain BSA115, (B) transcription is inducible by the addition of IPTG and negative control of (B) activity by the anti-sigma factor RsbW is absent. In contrast to our expectations of a continuous -galactosidase activity from a ctc::lacZ fusion, we observed a transient activity in the mutant. To explain this experimental finding, we constructed mathematical models reflecting different hypotheses regarding the regulation of (B) and -galactosidase dynamics. Only the model assuming instability of either ctc::lacZ mRNA or -galactosidase protein is able to reproduce the experiments in silico. Subsequent Northern blot experiments revealed stable high-level ctc::lacZ mRNA concentrations after the induction of the (B) response. Therefore, we conclude that protein instability following (B) activation is the most likely explanation for the experimental observations. Our results thus support the idea that B. subtilis increases the cytoplasmic proteolytic degradation to adapt the proteome in face of environmental challenges following activation of the general stress response. The findings also have practical implications for the analysis of stress response dynamics using lacZ reporter gene fusions, a frequently used strategy for the (B) response.

Figure 3a of the reference article has been reproduced. beta-galactosidase (lacz in model) activity at different concentrations of IPTG (100M, 200M and 1000M) has been reproduced. SED-ML (Simulation Experiment Description Markup Language) file is available for this model (see curation tab).

This model is hosted on BioModels Database and identifiedby: MODEL1212180000 .

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	compartment		3	1	litre	☑	

3.1 Compartment compartment

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

Name 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 7 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
IPTG	IPTG	compartment	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☑	☑
sigb	sigb	compartment	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☐
lacz	lacz	compartment	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☐
x	x	compartment	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☐

5 Parameters

This model contains six global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
kbd	kbd		0.044		☑
kbs	kbs		100.000		☑
kxd	kxd		9.000		☑
kxs	kxs		0.760		☑
kzd	kzd		0.041		☑
kzs	kzs		$4 \cdot 10^{-4}$		☑

6 Reactions

This model contains three 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	v1	v1	$\text{IPTG} \xrightleftharpoons{\text{IPTG, sigb}} \text{sigb}$	
2	v2	v2	$\text{sigb} \xrightleftharpoons{\text{x, lacz, sigb, x}} \text{lacz}$	
3	v3	v3	$\text{sigb} \xrightleftharpoons{\text{x, sigb}} \text{x}$	

6.1 Reaction v1

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

Name v1

Reaction equation

$$\text{IPTG} \xrightleftharpoons{\text{IPTG, sigb}} \text{sigb} \tag{1}$$

Reactant

Table 6: Properties of each reactant.

Id	Name	SBO
IPTG	IPTG	

Modifiers

Table 7: Properties of each modifier.

Id	Name	SBO
IPTG	IPTG	
sigb	sigb	

Product

Table 8: Properties of each product.

Id	Name	SBO
sigb	sigb	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = [\text{IPTG}] \cdot \text{kbs} - \text{kbd} \cdot [\text{sigb}] \tag{2}$$

6.2 Reaction v2

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

Name v2

Reaction equation

$$\text{sigb} \xrightleftharpoons{\text{x, lacz, sigb, x}} \text{lacz} \tag{3}$$

Reactant

Table 9: Properties of each reactant.

Id	Name	SBO
sigb	sigb	

Modifiers

Table 10: Properties of each modifier.

Id	Name	SBO
x	x	
lacz	lacz	
sigb	sigb	
x	x	

Product

Table 11: Properties of each product.

Id	Name	SBO
lacz	lacz	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = (\text{kzd} \cdot [\text{lacz}]) + \frac{\text{kzs} \cdot [\text{sigb}]}{1 + [\text{x}]} \tag{4}$$

6.3 Reaction v3

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

Name v3

Reaction equation

$$\text{sigb} \underset{}{\overset{\text{x, sigb}}{\rightleftharpoons}} \text{x} \tag{5}$$

Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
sigb	sigb	

Modifiers

Table 13: Properties of each modifier.

Id	Name	SBO
x	x	
sigb	sigb	

Product

Table 14: Properties of each product.

Id	Name	SBO
x	x	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = (\text{kxd} \cdot [\text{x}]) + \frac{\text{kxs} \cdot [\text{sigb}]}{1 + [\text{x}]} \tag{6}$$

7 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.

7.1 Species `IPTG`

Name IPTG

Initial concentration $100\ \mathrm{mol} \cdot \mathrm{l}^{-1}$

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:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{IPTG} = 0 \tag{7}$$

7.2 Species `sigb`

Name sigb

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

This species takes part in six reactions (as a reactant in `v2`, `v3` and as a product in `v1` and as a modifier in `v1`, `v2`, `v3`).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{sigb} = v_1 - v_2 - v_3 \tag{8}$$

7.3 Species `lacz`

Name lacz

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

This species takes part in two reactions (as a product in `v2` and as a modifier in `v2`).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{lacz} = v_2 \tag{9}$$

7.4 Species `x`

Name x

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

This species takes part in four reactions (as a product in `v3` and as a modifier in `v2`, `v2`, `v3`).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{x} = v_3 \tag{10}$$

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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