SBML Model Report

Model name: “Saeidi2012 - Quorum sensing device that produces GFP”

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 Nazanin Saeidi[2] at February 27th 2013 at 1:22 p. m. and last time modified at April eighth 2016 at 5:23 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	10
events	0	constraints	0
reactions	7	function definitions	0
global parameters	0	unit definitions	5
rules	0	initial assignments	0

Model Notes

Saeidi2012 - Quorum sensing device that produces GFP

Saeidi et al. (2012) has modelled a quorum sensing device that produces green fluorescent protein (GFP) as reporter in the presence of Acyl Homoserine Lactone (AHL).

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This model is described in the article:Characterization of a quorum sensing device for synthetic biology design: Experimental and modeling validationNazanin Saeidi, Mohamed Arshath, Matthew Wook Chang, Chueh Loo PohChemical Engineering Science. December 2012.

Abstract:

Modeling of biological parts is of crucial importance as it enables the in silico study of synthetic biological systems prior to the actual construction of genetic circuits, which can be time consuming and costly. Because standard biological parts are utilized to build the synthetic systems, it is important that each of these standard parts is well characterized and has a corresponding mathematical model that could simulate the characteristics of the part. These models could be used in computer aided design (CAD) tools during the design stage to facilitate the building of the model of biological systems. This paper describes the development of a mathematical model that is able to simulate both the dynamic and static performance of a biological device created using standard parts. We modeled an example quorum sensing device that produces green fluorescent protein (GFP) as reporter in the presence of Acyl Homoserine Lactone (AHL). The parameters of the model were estimated using experimental results. The simulation results show that the model was able to simulate behavior similar to experimental results. Since it is important that these models and the content in the models can be searchable and readable by machines, standard SBML (system biology markup language) format was used to store the models. All parts and reactions are fully annotated to enable easy searching, and the models follow the Minimum Information Requested In the Annotation of Models (MIRIAM) compliance as well as the Minimum Information About a Simulation Experiment (MIASE).

Figure 4a of the reference publication has been reproduced as curation figure. The plot shows the performance of the model at different concentrations of the inducer (3OC12HSL=5E-10, 5E-07, 5E-07).

This model is hosted on BioModels Database and identifiedby: MODEL1301110000 .

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.

2.1 Unit `substance`

Name substance

Definition mol

2.2 Unit `volume`

Name volume

Definition l

2.3 Unit `area`

Name area

Definition m^2

2.4 Unit `length`

Name length

Definition m

2.5 Unit `time`

Name 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
`default`			3	1	litre	☑	

3.1 Compartment `default`

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

4 Species

This model contains ten species. 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
s1	Ptet-LasR	default	mol	⊟	⊟
s19	LasR	default	mol	⊟	⊟
s3	sa3_degraded	default	mol	⊟	⊟
s4	3OC12HSL	default	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
s16	pLuxR	default	mol	⊟	⊟
s17	A pLux	default	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
s5	sa6_degraded	default	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
s42	LasR/AHL	default	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
s2	mRNA(LasR)	default	mol	⊟	⊟
s45	GFP	default	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟

5 Reactions

This model contains seven 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	re3		$s19 \xrightarrow{s19} s3$	
2	re2		$s2 \xrightarrow{s2} s19$	
3	re4		$s19 + s4 \xrightarrow{s19,\ s4,\ s42} s42$	
4	re5		$s42 + s16 \xrightarrow{s16,\ s42,\ s17} s17$	
5	re8		$s4 \xrightarrow{s4} s5$	
6	re1		$s1 \xrightarrow{s1,\ s2} s2$	
7	re14		$s17 \xrightarrow{s17,\ s45} s45$	

5.1 Reaction re3

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

Reaction equation

$$\mathrm{s19} \xrightarrow{\mathrm{s19}} \mathrm{s3} \tag{1}$$

Reactant

Table 5: Properties of each reactant.

Id	Name	SBO
s19	LasR	

Modifier

Table 6: Properties of each modifier.

Id	Name	SBO
s19	LasR	

Product

Table 7: Properties of each product.

Id	Name	SBO
s3	sa3_degraded	

Kinetic Law

Derived unit mol^2

$$v_1 = \mathrm{Y2} \cdot \mathrm{s19} \tag{2}$$

Table 8: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Y2	degradation rate of LasR		0.070	mol	☑

5.2 Reaction re2

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

Reaction equation

$$\mathrm{s2} \xrightarrow{\mathrm{s2}} \mathrm{s19} \tag{3}$$

Reactant

Table 9: Properties of each reactant.

Id	Name	SBO
s2	mRNA(LasR)	

Modifier

Table 10: Properties of each modifier.

Id	Name	SBO
s2	mRNA(LasR)	

Product

Table 11: Properties of each product.

Id	Name	SBO
s19	LasR	

Kinetic Law

Derived unit mol^2

$$v_2 = \mathrm{k2} \cdot \mathrm{s2} \tag{4}$$

Table 12: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k2	k2		35.7	mol	☑

5.3 Reaction re4

This is an irreversible reaction of two reactants forming one product influenced by three modifiers.

Reaction equation

$$\mathrm{s19} + \mathrm{s4} \xrightarrow{\mathrm{s19,\ s4,\ s42}} \mathrm{s42} \tag{5}$$

Reactants

Table 13: Properties of each reactant.

Id	Name	SBO
s19	LasR	
s4	3OC12HSL	

Modifiers

Table 14: Properties of each modifier.

Id	Name	SBO
s19	LasR	
s4	3OC12HSL	
s42	LasR/AHL	

Product

Table 15: Properties of each product.

Id	Name	SBO
s42	LasR/AHL	

Kinetic Law

Derived unit $\mathrm{mol}^3 \cdot \mathrm{l}^{-1}$

$$v_3 = \mathrm{s19} \cdot [\mathrm{s4}] \cdot \mathrm{k3} - \mathrm{k4} \cdot [\mathrm{s42}] \tag{6}$$

Table 16: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k3	k3		9600000.0	mol	☑
k4	k4		0.0	mol	☑

5.4 Reaction re5

This is an irreversible reaction of two reactants forming one product influenced by three modifiers.

Reaction equation

$$\mathrm{s42} + \mathrm{s16} \xrightarrow{\mathrm{s16,\ s42,\ s17}} \mathrm{s17} \tag{7}$$

Reactants

Table 17: Properties of each reactant.

Id	Name	SBO
s42	LasR/AHL	
s16	pLuxR	

Modifiers

Table 18: Properties of each modifier.

Id	Name	SBO
s16	pLuxR	
s42	LasR/AHL	
s17	A pLux	

Product

Table 19: Properties of each product.

Id	Name	SBO
s17	A pLux	

Kinetic Law

Derived unit $\mathrm{mol}^3 \cdot \mathrm{l}^{-1}$

$$v_4 = \mathrm{s16} \cdot [\mathrm{s42}] \cdot \mathrm{k5} - \mathrm{k6} \cdot [\mathrm{s17}] \tag{8}$$

Table 20: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k5	k5		1960000.0	mol	☑
k6	k6		10.2	mol	☑

5.5 Reaction re8

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

Reaction equation

$$\mathrm{s4} \xrightarrow{\mathrm{s4}} \mathrm{s5} \tag{9}$$

Reactant

Table 21: Properties of each reactant.

Id	Name	SBO
s4	3OC12HSL	

Modifier

Table 22: Properties of each modifier.

Id	Name	SBO
s4	3OC12HSL	

Product

Table 23: Properties of each product.

Id	Name	SBO
s5	sa6_degraded	

Kinetic Law

Derived unit $\mathrm{mol}^2 \cdot \mathrm{l}^{-1}$

$$v_5 = \mathrm{Y3} \cdot [\mathrm{s4}] \tag{10}$$

Table 24: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Y3	Y3		$2.832 \cdot 10^{-4}$	mol	☑

5.6 Reaction re1

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

Reaction equation

$$\mathrm{s1} \xrightarrow{\mathrm{s1,\ s2}} \mathrm{s2} \tag{11}$$

Reactant

Table 25: Properties of each reactant.

Id	Name	SBO
s1	Ptet-LasR	

Modifiers

Table 26: Properties of each modifier.

Id	Name	SBO
s1	Ptet-LasR	
s2	mRNA(LasR)	

Product

Table 27: Properties of each product.

Id	Name	SBO
s2	mRNA(LasR)	

Kinetic Law

Derived unit mol^2

$$v_6 = \mathrm{k1} \cdot \mathrm{s1} - \mathrm{Y1} \cdot \mathrm{s2} \tag{12}$$

Table 28: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	k1		3.734	mol	☑
Y1	Y1		0.348	mol	☑

5.7 Reaction re14

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

Reaction equation

$$\mathrm{s17} \xrightarrow{\mathrm{s17,\ s45}} \mathrm{s45} \tag{13}$$

Reactant

Table 29: Properties of each reactant.

Id	Name	SBO
s17	A pLux	

Modifiers

Table 30: Properties of each modifier.

Id	Name	SBO
s17	A pLux	
s45	GFP	

Product

Table 31: Properties of each product.

Id	Name	SBO
s45	GFP	

Kinetic Law

Derived unit mol^2

$$v_7 = \left(\mathrm{K7} + \frac{\mathrm{K8} \cdot [\mathrm{s17}]^{\mathrm{n1}}}{\mathrm{K9}^{\mathrm{n1}} + [\mathrm{s17}]^{\mathrm{n1}}}\right) \cdot \left(\mathrm{k10} + \frac{\mathrm{K11} \cdot [\mathrm{s17}]^{\mathrm{n2}}}{\mathrm{K12}^{\mathrm{n2}} + [\mathrm{s17}]^{\mathrm{n2}}} - [\mathrm{s45}]\right) \tag{14}$$

Table 32: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
K7	K7		0.004	mol	☑
K8	K8		0.010	mol	☑
K9	K9		$9.742 \cdot 10^{-8}$	mol	☑
k10	K10		$6.5 \cdot 10^{-16}$	mol	☑
K11	K11		10^{-14}	mol	☑
K12	K12		$2.4 \cdot 10^{-7}$	mol	☑
n1	n1		2.000	mol	☑
n2	n2		2.000	mol	☑

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 s1

Name Ptet-LasR

Initial amount 10^{-5} mol

Charge 0

This species takes part in two reactions (as a reactant in re1 and as a modifier in re1).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s1} = -v_6 \tag{15}$$

6.2 Species s19

Name LasR

Initial amount 10^{-6} mol

Charge 0

This species takes part in five reactions (as a reactant in re3, re4 and as a product in re2 and as a modifier in re3, re4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s19} = v_2 - v_1 - v_3 \tag{16}$$

6.3 Species s3

Name sa3_degraded

Initial amount 0 mol

Charge 0

This species takes part in one reaction (as a product in re3).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s3} = v_1 \tag{17}$$

6.4 Species s4

Name 3OC12HSL

Initial concentration $5 \cdot 10^{-6}$ mol$\cdot$l^{-1}

Charge 0

This species takes part in four reactions (as a reactant in re4, re8 and as a modifier in re4, re8).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s4} = -v_3 - v_5 \tag{18}$$

6.5 Species s16

Name pLuxR

Initial amount 10^{-5} mol

Charge 0

This species takes part in two reactions (as a reactant in re5 and as a modifier in re5).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s16} = -\,v_4 \tag{19}$$

6.6 Species s17

Name A pLux

Initial amount 0 mol

Charge 0

This species takes part in four reactions (as a reactant in re14 and as a product in re5 and as a modifier in re5, re14).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s17} = v_4 - v_7 \tag{20}$$

6.7 Species s5

Name sa6_degraded

Initial amount 0 mol

This species takes part in one reaction (as a product in re8).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s5} = v_5 \tag{21}$$

6.8 Species s42

Name LasR/AHL

Initial amount 0 mol

This species takes part in four reactions (as a reactant in re5 and as a product in re4 and as a modifier in re4, re5).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s42} = v_3 - v_4 \tag{22}$$

6.9 Species s2

Name mRNA(LasR)

Initial amount 0 mol

Charge 0

This species takes part in four reactions (as a reactant in re2 and as a product in re1 and as a modifier in re2, re1).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s2} = v_6 - v_2 \tag{23}$$

6.10 Species s45

Name GFP

Initial amount 0 mol

This species takes part in two reactions (as a product in re14 and as a modifier in re14).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s45} = v_7 \tag{24}$$

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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