SBML Model Report

Model name: "Balagadd2008_E_coli_Predator_Prey"

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1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by the following two authors: Lukas Endler[1] and Hao Song[2] at January twelveth 2011 at 2:16 a. m. and last time modified at April first 2014 at 2:29 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	7
events	0	constraints	0
reactions	8	function definitions	0
global parameters	12	unit definitions	2
rules	2	initial assignments	0

Model Notes

This is the reduced model described in the article:
A synthetic Escherichia coli predatorprey ecosystem

[1]EMBL-EBI, lukas@ebi.ac.uk
[2]Department of Biomedical Engineering and Institute for Genome Sciences and Policy, Duke University, hs59@duke.edu

Balagadd FK, Song H, Ozaki J, Collins CH, Barnet M, Arnold FH, Quake SR, You L.Mol Syst Biol. 2008;4:187. Epub 2008 Apr 15. PMID: 18414488; DOI:10.1038/msb.2008.24

Abstract:
We have constructed a synthetic ecosystem consisting of two Escherichia coli populations, which communicate bi-directionally through quorum sensing and regulate each other's gene expression and survival via engineered gene circuits. Our synthetic ecosystem resembles canonical predatorprey systems in terms of logic and dynamics. The predator cells kill the prey by inducing expression of a killer protein in the prey, while the prey rescue the predators by eliciting expression of an antidote protein in the predator. Extinction, coexistence and oscillatory dynamics of the predator and prey populations are possible depending on the operating conditions as experimentally validated by long-term culturing of the system in microchemostats. A simple mathematical model is developed to capture these system dynamics. Coherent interplay between experiments and mathematical analysis enables exploration of the dynamics of interacting populations in a predictable manner.

In the article the cell density is given in per 10^3 cells per microlitre. To evade a conversion factor in the SBML implementation, the unit for the cell densities was just left the same as for the AHLs A and A2 (nM).

2 Unit Definitions

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

2.1 Unit `substance`

Name nanomole

Definition nmol

2.2 Unit `time`

Name hours

Definition 3600 s

2.3 Unit volume

Notes Litre is the predefined SBML unit for volume.

Definition l

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
environment		0000290	3	1	litre	☑	

3.1 Compartment environment

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

SBO:0000290 physical compartment

4 Species

This model contains seven species. The boundary condition of two of these species is set to `true` so that these species' amount cannot be changed by any reaction. 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
IPTG		environment	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	☑	☐
C1		environment	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	☐	☐
C2		environment	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	☐	☐
A1		environment	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	☐	☐
A2		environment	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	☐	☐
sink		environment	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	☐	☑
source		environment	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	☐	☑

5 Parameters

This model contains twelve global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
kc1		0000035	0.800		☑
kc2		0000035	0.400		☑
Cm		0000196	100.000		☑
D		0000356	0.113		☑
kA1		0000035	0.100		☑
kA2		0000035	0.000		☐
d2		0000356	0.300		☑
K2		0000191	10.000		☑
d1		0000356	0.000		☐
K1		0000191	10.000		☑
dAA1		0000356	0.017		☑
dAA2		0000356	0.110		☑

6 Rules

This is an overview of two rules.

6.1 Rule d1

Rule d1 is an assignment rule for parameter d1:

$$\mathrm{d1} = 0.5 + \frac{[\mathrm{IPTG}]^2}{5^2 + [\mathrm{IPTG}]^2} \tag{1}$$

6.2 Rule kA2

Rule kA2 is an assignment rule for parameter kA2:

$$\mathrm{kA2} = 0.02 + 0.03 \cdot \frac{[\mathrm{IPTG}]^2}{5^2 + [\mathrm{IPTG}]^2} \tag{2}$$

7 Reactions

This model contains eight 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	J0	predator growth	source $\xrightarrow{C2}$ C1	0000375
2	J1	predator death	C1 $\xrightarrow{A2}$ sink	0000179
3	J2	prey growth	source $\xrightarrow{C1}$ C2	0000375
4	J3	prey death	C2 $\xrightarrow{A1}$ sink	0000179
5	J4	3OC12HSL synthesis	source $\xrightarrow{C1}$ A1	0000205
6	J5	3OC12HSL removal	A1 $\longrightarrow$ sink	0000179
7	J6	3OC6HSL synthesis	source $\xrightarrow{C2}$ A2	0000205
8	J7	3OC6HSL removal	A2 $\longrightarrow$ sink	0000179

7.1 Reaction J0

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

Name predator growth

SBO:0000375 process

Reaction equation

$$\text{source} \xrightarrow{\text{C2}} \text{C1} \tag{3}$$

Reactant

Table 6: Properties of each reactant.

Id	Name	SBO
source		

Modifier

Table 7: Properties of each modifier.

Id	Name	SBO
C2		

Product

Table 8: Properties of each product.

Id	Name	SBO
C1		

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \text{vol}\,(\text{environment}) \cdot \text{kc1} \cdot [\text{C1}] \cdot \left(1 - \frac{[\text{C1}] + [\text{C2}]}{\text{Cm}}\right) \tag{4}$$

7.2 Reaction J1

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

Name predator death

SBO:0000179 degradation

Reaction equation

$$\mathrm{C1} \xrightarrow{\mathrm{A2}} \mathrm{sink} \tag{5}$$

Reactant

Table 9: Properties of each reactant.

Id	Name	SBO
C1		

Modifier

Table 10: Properties of each modifier.

Id	Name	SBO
A2		

Product

Table 11: Properties of each product.

Id	Name	SBO
sink		

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \mathrm{vol}\,(\mathrm{environment}) \cdot \left(\mathrm{D} + \frac{\mathrm{d1} \cdot \mathrm{K1}}{\mathrm{K1} + [\mathrm{A2}]^2}\right) \cdot [\mathrm{C1}] \tag{6}$$

7.3 Reaction J2

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

Name prey growth

SBO:0000375 process

Reaction equation

$$\text{source} \xrightarrow{\text{C1}} \text{C2} \tag{7}$$

Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
source		

Modifier

Table 13: Properties of each modifier.

Id	Name	SBO
C1		

Product

Table 14: Properties of each product.

Id	Name	SBO
C2		

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \text{vol}\,(\text{environment}) \cdot \text{kc2} \cdot [\text{C2}] \cdot \left(1 - \frac{[\text{C1}] + [\text{C2}]}{\text{Cm}}\right) \tag{8}$$

7.4 Reaction J3

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

Name prey death

SBO:0000179 degradation

Reaction equation

$$\text{C2} \xrightarrow{\text{A1}} \text{sink} \tag{9}$$

Reactant

Table 15: Properties of each reactant.

Id	Name	SBO
C2		

Modifier

Table 16: Properties of each modifier.

Id	Name	SBO
A1		

Product

Table 17: Properties of each product.

Id	Name	SBO
sink		

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \mathrm{vol}\,(\mathrm{environment}) \cdot \left(\mathrm{D} + \frac{\mathrm{d2} \cdot [\mathrm{A1}]^2}{\mathrm{K2} + [\mathrm{A1}]^2}\right) \cdot [\mathrm{C2}] \tag{10}$$

7.5 Reaction J4

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

Name 3OC12HSL synthesis

SBO:0000205 composite biochemical process

Reaction equation

$$\mathrm{source} \xrightarrow{\mathrm{C1}} \mathrm{A1} \tag{11}$$

Reactant

Table 18: Properties of each reactant.

Id	Name	SBO
source		

Modifier

Table 19: Properties of each modifier.

Id	Name	SBO
C1		

Product

Table 20: Properties of each product.

Id	Name	SBO
A1		

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \mathrm{vol}\,(\mathrm{environment}) \cdot \mathrm{kA1} \cdot [\mathrm{C1}] \tag{12}$$

7.6 Reaction J5

This is an irreversible reaction of one reactant forming one product.

Name 3OC12HSL removal

SBO:0000179 degradation

Reaction equation

$$\mathrm{A1} \longrightarrow \mathrm{sink} \tag{13}$$

Reactant

Table 21: Properties of each reactant.

Id	Name	SBO
A1		

Product

Table 22: Properties of each product.

Id	Name	SBO
sink		

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \text{vol}\,(\text{environment}) \cdot (\text{dAA1} + \text{D}) \cdot [\text{A1}] \tag{14}$$

7.7 Reaction J6

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

Name 3OC6HSL synthesis

SBO:0000205 composite biochemical process

Reaction equation

$$\text{source} \xrightarrow{\text{C2}} \text{A2} \tag{15}$$

Reactant

Table 23: Properties of each reactant.

Id	Name	SBO
source		

Modifier

Table 24: Properties of each modifier.

Id	Name	SBO
C2		

Product

Table 25: Properties of each product.

Id	Name	SBO
A2		

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \mathrm{vol}\,(\mathrm{environment}) \cdot \mathrm{kA2} \cdot [\mathrm{C2}] \tag{16}$$

7.8 Reaction J7

This is an irreversible reaction of one reactant forming one product.

Name 3OC6HSL removal

SBO:0000179 degradation

Reaction equation

$$\mathrm{A2} \longrightarrow \mathrm{sink} \tag{17}$$

Reactant

Table 26: Properties of each reactant.

Id	Name	SBO
A2		

Product

Table 27: Properties of each product.

Id	Name	SBO
sink		

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \text{vol}\,(\text{environment}) \cdot (\text{dAA2} + \text{D}) \cdot [\text{A2}] \tag{18}$$

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 `IPTG`

SBO:0000247 simple chemical

Notes IPTG default 5 nM

Initial concentration $5\ \text{nmol} \cdot \text{l}^{-1}$

$$\frac{\text{d}}{\text{d}t}\text{IPTG} = 0 \tag{19}$$

8.2 Species `C1`

SBO:0000240 material entity

Notes predator cells (MG1655) (per 10^3 cells per microlitre)

Initial concentration $20\ \text{nmol} \cdot \text{l}^{-1}$

This species takes part in four reactions (as a reactant in `J1` and as a product in `J0` and as a modifier in `J2`, `J4`).

$$\frac{\text{d}}{\text{d}t}\text{C1} = v_1 - v_2 \tag{20}$$

8.3 Species C2

SBO:0000240 material entity

Notes prey cells (Top10F) (per 10^3 cells per microlitre)

Initial concentration $20\ \mathrm{nmol \cdot l^{-1}}$

This species takes part in four reactions (as a reactant in J3 and as a product in J2 and as a modifier in J0, J6).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C2} = v_3 - v_4 \tag{21}$$

8.4 Species A1

SBO:0000247 simple chemical

Notes 3OC12HSL

Initial concentration $0.1\ \mathrm{nmol \cdot l^{-1}}$

This species takes part in three reactions (as a reactant in J5 and as a product in J4 and as a modifier in J3).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{A1} = v_5 - v_6 \tag{22}$$

8.5 Species A2

SBO:0000247 simple chemical

Notes 3OC6HSL

Initial concentration $0.1\ \mathrm{nmol \cdot l^{-1}}$

This species takes part in three reactions (as a reactant in J7 and as a product in J6 and as a modifier in J1).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{A2} = v_7 - v_8 \tag{23}$$

8.6 Species sink

SBO:0000291 empty set

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

This species takes part in four reactions (as a product in J1, J3, J5, J7), which do not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{sink} = 0 \tag{24}$$

8.7 Species `source`

SBO:0000291 empty set

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

This species takes part in four reactions (as a reactant in `J0`, `J2`, `J4`, `J6`), which do not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{source} = 0 \tag{25}$$

A Glossary of Systems Biology Ontology Terms

SBO:0000035 **forward unimolecular rate constant, continuous case:** Numerical parameter that quantifies the forward velocity of a chemical reaction involving only one reactant. This parameter encompasses all the contributions to the velocity except the quantity of the reactant. It is to be used in a reaction modelled using a continuous framework

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

SBO:0000191 **Hill constant:** Empirical constant created by Archibald Vivian Hill to describe the cooperative binding of oxygen on hemoglobine (Hill (1910). The possible effects of the aggregation of the molecules of haemoglobin on its dissociation curves. J Physiol 40: iv-vii). Different from a microscopic dissociation constant, it has the dimension of concentration to the power of the Hill coefficient

SBO:0000196 **concentration of an entity pool:** The amount of an entity per unit of volume.

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:0000240 **material entity:** A real thing that is defined by its physico-chemical structure.

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:0000291 **empty set:** Entity defined by the absence of any actual object. An empty set is often used to represent the source of a creation process or the result of a degradation process.

SBO:0000356 **decay constant:** Kinetic constant characterising a mono-exponential decay. It is the inverse of the mean lifetime of the continuant being decayed. Its unit is“per tim”.

SBO:0000375 **process:** A sequential series of actions, motions, or occurrences, such as chemical reactions, that affect one or more entities in a phenomenologically characteristic manner

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