SBML Model Report

Model name: “Boada2016 - Incoherent type 1 feed-forward loop (I1-FFL)”

May 17, 2018

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by Matthew Grant Roberts[1] at April 24th 2018 at 12:08 a. m. and last time modified at April 25th 2018 at 11:10 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	2
species types	0	species	9
events	0	constraints	0
reactions	23	function definitions	8
global parameters	41	unit definitions	2
rules	8	initial assignments	5

Model Notes

Boada2016 - Incoherent type 1 feed-forwardloop (I1-FFL)A synthetic-biology mathematicalmodelling framework that was constructed to provide guidelines forexperimental implementation and parameter optimisation resulted ina biological device demonstrating desired behaviour.

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This model is described in the article:Multi-objective optimization framework to obtain model-based guidelines for tuning biological synthetic devices: an adaptive network case.Boada Y, Reynoso-Meza G, Pic J, Vignoni A.BMC Syst Biol 2016 Mar; 10: 27

Abstract:

Model based design plays a fundamental role in synthetic biology. Exploiting modularity, i.e. using biological parts and interconnecting them to build new and more complex biological circuits is one of the key issues. In this context, mathematical models have been used to generate predictions of the behavior of the designed device. Designers not only want the ability to predict the circuit behavior once all its components have been determined, but also to help on the design and selection of its biological parts, i.e. to provide guidelines for the experimental implementation. This is tantamount to obtaining proper values of the model parameters, for the circuit behavior results from the interplay between model structure and parameters tuning. However, determining crisp values for parameters of the involved parts is not a realistic approach. Uncertainty is ubiquitous to biology, and the characterization of biological parts is not exempt from it. Moreover, the desired dynamical behavior for the designed circuit usually results from a trade-off among several goals to be optimized.We propose the use of a multi-objective optimization tuning framework to get a model-based set of guidelines for the selection of the kinetic parameters required to build a biological device with desired behavior. The design criteria are encoded in the formulation of the objectives and optimization problem itself. As a result, on the one hand the designer obtains qualitative regions/intervals of values of the circuit parameters giving rise to the predefined circuit behavior; on the other hand, he obtains useful information for its guidance in the implementation process. These parameters are chosen so that they can effectively be tuned at the wet-lab, i.e. they are effective biological tuning knobs. To show the proposed approach, the methodology is applied to the design of a well known biological circuit: a genetic incoherent feed-forward circuit showing adaptive behavior.The proposed multi-objective optimization design framework is able to provide effective guidelines to tune biological parameters so as to achieve a desired circuit behavior. Moreover, it is easy to analyze the impact of the context on the synthetic device to be designed. That is, one can analyze how the presence of a downstream load influences the performance of the designed circuit, and take it into account.

This model is hosted on BioModels Database and identified by: BIOMD0000000696.

To cite BioModels Database, please use: Chelliah V et al. BioModels: ten-year anniversary. Nucl. Acids Res. 2015, 43(Database issue):D542-8.

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 volume

Name volume

Definition µl

2.2 Unit substance

Name substance

Definition nmol

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 Compartments

This model contains two compartments.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
Cell	Cell		3	1	litre	☑	
Extracellular	Extracellular		3	1	litre	☑	

3.1 Compartment Cell

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

Name Cell

Notes `Original encoded model had volume set to 0.0432 ul`

3.2 Compartment `Extracellular`

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

Name Extracellular

Notes `Original encoded model had volume set to 180 ul`

4 Species

This model contains nine species. 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
x1	x1	Cell	$\mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$	⊟	⊟
x2	x2	Cell	$\mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$	⊟	⊟
x3	x3	Cell	$\mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$	⊟	⊟
x4	x4	Cell	$\mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$	⊟	⊟
x5	x5	Cell	$\mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$	⊟	⊟
x6	x6	Cell	$\mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$	⊟	⊟
x7	x7	Cell	$\mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$	⊟	⊟
x8	x8	Cell	$\mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$	⊟	⊟
x9	x9	Extracellular	$\mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$	⊟	⊟

5 Parameters

This model contains 41 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k_mA_C_gA	k_mA*C_gA		104.000		☑
k_mB_C_gB	k_mB*C_gB		1.000		☑
k_mC_C_gC	k_mC*C_gC		1.000		☑
d_mA	d_mA		0.362		☑
d_mB	d_mB		0.362		☑
d_mC	d_mC		0.362		☑
k_pA	k_pA		80.000		☑
k_pB	k_pB		1.000		☑
k_pC	k_pC		11.420		☑
d_A	d_A		0.035		☑
d_B	d_B		0.016		☑
d_C	d_C		0.278		☑
k_d	k_d		0.060		☑
k_2f	k_2f		0.100		☑
k_3f	k_3f		0.100		☑
k_2r	k_2r		20.000		☑
k_3r	k_3r		1.000		☑
gamma_1	gamma_1		107.400		☑
gamma_2	gamma_2		0.200		☑
gamma_3	gamma_3		0.010		☑
gamma_4	gamma_4		1.150		☑
gamma_5	gamma_5		8.560		☑
Beta_1	Beta_1		0.050		☑
Beta_2	Beta_2		0.050		☑
d_I	d_I		0.016		☑
d_Ie	d_Ie		0.016		☑
d_AI	d_AI		0.035		☑
d_AI2	d_AI2		0.035		☑
M	M		0.000		☐
K_cells	K_cells		$1.33333333333333 \cdot 10^{-9}$		☐
V_cell	V_cell		10^{-15}		☑
N_cells	N_cells		$2.4 \cdot 10^{8}$		☑
V_medium	V_medium		180.000		☑
sum_abs_dx8	sum(abs_dx8)		0.000		☐
J1	J1		0.000		☐
J2	J2		0.000		☐

Id	Name	SBO	Value	Unit	Constant
Sensitivity	Sensitivity		0.000		☐
Precision	Precision		0.000		☐
P_theta	P_theta		0.000		☐
Metabolite_16	Initial for x8		0.000		☑
Metabolite_17	Initial for x9		9000.000		☑

6 Initialassignments

This is an overview of five initialassignments.

6.1 Initialassignment x1

Derived unit contains undeclared units

Math $\frac{0.0432 \cdot 104}{0.3624}$

6.2 Initialassignment x2

Derived unit contains undeclared units

Math $\frac{0.0432 \cdot 104 \cdot 80}{0.3624 \cdot 0.035}$

6.3 Initialassignment x9

Derived unit contains undeclared units

Math $50 \cdot 180$

6.4 Initialassignment Metabolite_16

Derived unit $\mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$

Math [x8]

6.5 Initialassignment Metabolite_17

Derived unit $\mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$

Math [x9]

7 Function definitions

This is an overview of eight function definitions.

7.1 Function definition rateOf

Argument a

Mathematical Expression

$$NaN \tag{1}$$

7.2 Function definition Constant_flux__irreversible

Name Constant flux (irreversible)

Argument v

Mathematical Expression

$$\mathrm{v} \tag{2}$$

7.3 Function definition function_for_r014___C_translation

Name function for r014 - C_translation

Arguments KmCCgC, [x4], Beta1, gamma4, [x6], Beta2, gamma5, gamma2, gamma3

Mathematical Expression

$$\mathrm{KmCCgC} \cdot \frac{[\mathrm{x4}] + \mathrm{Beta1} \cdot \mathrm{gamma4} \cdot [\mathrm{x6}] + \mathrm{Beta2} \cdot \mathrm{gamma5} \cdot [\mathrm{x4}] \cdot [\mathrm{x6}]}{\mathrm{gamma2} + \mathrm{gamma3} \cdot [\mathrm{x4}] + \mathrm{gamma4} \cdot [\mathrm{x6}] + \mathrm{gamma5} \cdot [\mathrm{x4}] \cdot [\mathrm{x6}]} \tag{3}$$

7.4 Function definition function_for_r020___AI2_dim_4

Name function for r020 - AI2_dim_4

Arguments k3, M

Mathematical Expression

$$\mathrm{k3} \cdot \mathrm{M} \cdot \mathrm{M} \tag{4}$$

7.5 Function definition function_for_r019___AI2_dim_3

Name function for r019 - AI2_dim_3

Arguments k_2r, M

Mathematical Expression

$$\mathrm{k\_2r} \cdot \mathrm{M} \tag{5}$$

7.6 Function definition function_for_r006d

Name function for r006d

Arguments Kcells, kd, [x3]

Mathematical Expression

$$\text{Kcells} \cdot \text{kd} \cdot [\text{x3}] \tag{6}$$

7.7 Function definition function_for_r010___x5_transcription

Name function for r010 - x5 transcription

Arguments K_mbC_gB, [x4], gamma1

Mathematical Expression

$$\text{K\_mbC\_gB} \cdot \frac{[\text{x4}]}{\text{gamma1} + [\text{x4}]} \tag{7}$$

7.8 Function definition function_for_r006c

Name function for r006c

Arguments Kcells, kd, [x9]

Mathematical Expression

$$\text{Kcells} \cdot \text{kd} \cdot [\text{x9}] \tag{8}$$

8 Rules

This is an overview of eight rules.

8.1 Rule J1

Rule J1 is an assignment rule for parameter J1:

$$\text{J1} = \frac{2 \cdot |[\text{x9}] - \text{Metabolite\_17}|}{\text{sum\_abs\_dx8}} \tag{9}$$

8.2 Rule Sensitivity

Rule Sensitivity is an assignment rule for parameter Sensitivity:

$$\text{Sensitivity} = \frac{1}{\text{J1}} \tag{10}$$

8.3 Rule J2

Rule J2 is an assignment rule for parameter J2:

$$\mathrm{J2} = \frac{[\mathrm{x8}] - \mathrm{Metabolite\_16}}{[\mathrm{x9}] - \mathrm{Metabolite\_17}} \tag{11}$$

8.4 Rule Precision

Rule Precision is an assignment rule for parameter Precision:

$$\mathrm{Precision} = \frac{1}{\mathrm{J2}} \tag{12}$$

8.5 Rule M

Rule M is an assignment rule for parameter M:

$$\mathrm{M} = \left(\frac{\mathrm{d\_AI} + \mathrm{k\_2r}}{4 \cdot \mathrm{k\_3f}}\right) + \frac{1}{4 \cdot \mathrm{k\_3f}} \cdot \sqrt{2} \tag{13}$$

8.6 Rule K_cells

Rule K_cells is an assignment rule for parameter K_cells:

$$\mathrm{K\_cells} = \frac{\mathrm{V\_cell} \cdot \mathrm{N\_cells}}{\mathrm{V\_medium}} \tag{14}$$

8.7 Rule sum_abs_dx8

Rule sum_abs_dx8 is a rate rule for parameter sum_abs_dx8:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{sum\_abs\_dx8} = |\mathrm{rateOf}([\mathrm{x8}])| \tag{15}$$

8.8 Rule P_theta

Rule P_theta is a rate rule for parameter P_theta:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{P\_theta} = |\mathrm{rateOf}([\mathrm{x6}])| \tag{16}$$

9 Reactions

This model contains 23 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	r001___mA_transcription	r001 - mA_transcription	$\emptyset \longrightarrow x1$	
2	r002___A_translation	r002 - A_translation	$x1 \longrightarrow x1 + x2$	
3	r003___mA_degradation	r003 - mA_degradation	$x1 \longrightarrow \emptyset$	
4	r004___A_degradation	r004 - A_degradation	$x2 \longrightarrow \emptyset$	
5	r005___AI2_dim_1	r005 - AI2_dim_1	$x2 + x3 \longrightarrow \emptyset$	
6	r006a___I_transport	r006a - I_transport	$x3 \longrightarrow \emptyset$	
7	r007___I_degradation	r007 - I_degradation	$x3 \longrightarrow \emptyset$	
8	r008___Ie_degradation	r008 - Ie_degradation	$x9 \longrightarrow \emptyset$	
9	r009___AI2_degradation	r009 - AI2_degradation	$x4 \longrightarrow \emptyset$	
10	r010___mB_transcription	r010 - mB_transcription	$\emptyset \xrightarrow{x4} x5$	
11	r011___B_translation	r011 - B_translation	$x5 \longrightarrow x5 + x6$	

№	Id	Name	Reaction Equation	SBO
12	r012___B-_degradation	r012 - B_degradation	$x6 \longrightarrow \emptyset$	
13	r013___mB-_degradation	r013 - mB_degradation	$x5 \longrightarrow \emptyset$	
14	r014___mC-_transcription	r014 - mC_transcription	$\emptyset \xrightarrow{x4,\ x6} x7$	
15	r015___C-_translation	r015 - C_translation	$x7 \longrightarrow x7 + x8$	
16	r016___C-_degradation	r016 - C_degradation	$x8 \longrightarrow \emptyset$	
17	r017___mC-_degradation	r017 - mC_degradation	$x7 \longrightarrow \emptyset$	
18	r018___AI2_dim_2	r018 - AI2_dim_2	$x4 \longrightarrow \emptyset$	
19	r019___AI2_dim_3	r019 - AI2_dim_3	$\emptyset \longrightarrow x2 + x3$	
20	r020___AI2_dim_4	r020 - AI2_dim_4	$\emptyset \longrightarrow x4$	
21	r006b___I-_transport	r006b - I_transport	$x9 \longrightarrow x9 + x3$	
22	r006c___I-_transport	r006c - I_transport	$x9 \longrightarrow \emptyset$	
23	r006d___I-_transport	r006d - I_transport	$\emptyset \xrightarrow{x3} x9$	

9.1 Reaction r001___mA_transcription

This is an irreversible reaction of no reactant forming one product.

Name r001 - mA_transcription

Reaction equation

$$\emptyset \longrightarrow \mathrm{x1} \tag{17}$$

Product

Table 6: Properties of each product.

Id	Name	SBO
x1	x1	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \mathrm{vol}\left(\mathrm{Cell}\right) \cdot \mathrm{Constant\_flux\_\_irreversible}\left(\mathrm{k\_mA\_C\_gA}\right) \tag{18}$$

$$\mathrm{Constant\_flux\_\_irreversible}\left(\mathrm{v}\right) = \mathrm{v} \tag{19}$$

$$\mathrm{Constant\_flux\_\_irreversible}\left(\mathrm{v}\right) = \mathrm{v} \tag{20}$$

9.2 Reaction r002___A_translation

This is an irreversible reaction of one reactant forming two products.

Name r002 - A_translation

Reaction equation

$$\mathrm{x1} \longrightarrow \mathrm{x1} + \mathrm{x2} \tag{21}$$

Reactant

Table 7: Properties of each reactant.

Id	Name	SBO
x1	x1	

Products

Table 8: Properties of each product.

Id	Name	SBO
x1	x1	
x2	x2	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \mathrm{vol}\,(\mathrm{Cell}) \cdot \mathrm{k\_pA} \cdot [\mathrm{x1}] \tag{22}$$

9.3 Reaction r003__mA_degradation

This is an irreversible reaction of one reactant forming no product.

Name r003 - mA_degradation

Reaction equation

$$\mathrm{x1} \longrightarrow \emptyset \tag{23}$$

Reactant

Table 9: Properties of each reactant.

Id	Name	SBO
x1	x1	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \mathrm{vol}\,(\mathrm{Cell}) \cdot \mathrm{d\_mA} \cdot [\mathrm{x1}] \tag{24}$$

9.4 Reaction r004___A_degradation

This is an irreversible reaction of one reactant forming no product.

Name r004 - A_degradation

Reaction equation

$$\mathrm{x2} \longrightarrow \emptyset \tag{25}$$

Reactant

Table 10: Properties of each reactant.

Id	Name	SBO
x2	x2	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \mathrm{vol}\,(\mathrm{Cell}) \cdot \mathrm{d\_A} \cdot [\mathrm{x2}] \tag{26}$$

9.5 Reaction r005___AI2_dim_1

This is an irreversible reaction of two reactants forming no product.

Name r005 - AI2_dim_1

Reaction equation

$$\mathrm{x2} + \mathrm{x3} \longrightarrow \emptyset \tag{27}$$

Reactants

Table 11: Properties of each reactant.

Id	Name	SBO
x2	x2	
x3	x3	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \mathrm{vol}\,(\mathrm{Cell}) \cdot \mathrm{k\_2f} \cdot [\mathrm{x2}] \cdot [\mathrm{x3}] \tag{28}$$

9.6 Reaction r006a___I_transport

This is an irreversible reaction of one reactant forming no product.

Name r006a - I_transport

Reaction equation

$$\mathrm{x3} \longrightarrow \emptyset \tag{29}$$

Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
x3	x3	

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \mathrm{vol}\,(\mathrm{Cell}) \cdot \mathrm{k\_d} \cdot [\mathrm{x3}] \tag{30}$$

9.7 Reaction r007___I_degradation

This is an irreversible reaction of one reactant forming no product.

Name r007 - I_degradation

Reaction equation

$$\mathrm{x3} \longrightarrow \emptyset \tag{31}$$

Reactant

Table 13: Properties of each reactant.

Id	Name	SBO
x3	x3	

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \mathrm{vol}\,(\mathrm{Cell}) \cdot \mathrm{d\_I} \cdot [\mathrm{x3}] \tag{32}$$

9.8 Reaction r008___Ie_degradation

This is an irreversible reaction of one reactant forming no product.

Name r008 - Ie_degradation

Reaction equation

$$\mathrm{x9} \longrightarrow \emptyset \tag{33}$$

Reactant

Table 14: Properties of each reactant.

Id	Name	SBO
x9	x9	

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \mathrm{vol}\,(\mathrm{Extracellular}) \cdot \mathrm{d\_Ie} \cdot [\mathrm{x9}] \tag{34}$$

9.9 Reaction r009___AI2_degradation

This is an irreversible reaction of one reactant forming no product.

Name r009 - AI2_degradation

Reaction equation

$$\mathrm{x4} \longrightarrow \emptyset \tag{35}$$

Reactant

Table 15: Properties of each reactant.

Id	Name	SBO
x4	x4	

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \mathrm{vol}\,(\mathrm{Cell}) \cdot \mathrm{d\_AI2} \cdot [\mathrm{x4}] \tag{36}$$

9.10 Reaction r010___mB_transcription

This is an irreversible reaction of no reactant forming one product influenced by one modifier.

Name r010 - mB_transcription

Reaction equation

$$\emptyset \xrightarrow{\mathrm{x4}} \mathrm{x5} \tag{37}$$

Modifier

Table 16: Properties of each modifier.

Id	Name	SBO
x4	x4	

Product

Table 17: Properties of each product.

Id	Name	SBO
x5	x5	

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = \mathrm{vol}\,(\mathrm{Cell}) \cdot \mathrm{function\_for\_r010\_\_\_x5\_transcription}\,(\mathrm{k\_mB\_C\_gB}, [\mathrm{x4}], \mathrm{gamma\_1}) \quad (38)$$

$$\mathrm{function\_for\_r010\_\_\_x5\_transcription}\,(\mathrm{K\_mbC\_gB}, [\mathrm{x4}], \mathrm{gamma1}) = \mathrm{K\_mbC\_gB} \cdot \frac{[\mathrm{x4}]}{\mathrm{gamma1} + [\mathrm{x4}]} \quad (39)$$

$$\mathrm{function\_for\_r010\_\_\_x5\_transcription}\,(\mathrm{K\_mbC\_gB}, [\mathrm{x4}], \mathrm{gamma1}) = \mathrm{K\_mbC\_gB} \cdot \frac{[\mathrm{x4}]}{\mathrm{gamma1} + [\mathrm{x4}]} \quad (40)$$

9.11 Reaction r011___B_translation

This is an irreversible reaction of one reactant forming two products.

Name r011 - B_translation

Reaction equation

$$\mathrm{x5} \longrightarrow \mathrm{x5} + \mathrm{x6} \quad (41)$$

Reactant

Table 18: Properties of each reactant.

Id	Name	SBO
x5	x5	

Products

Table 19: Properties of each product.

Id	Name	SBO
x5	x5	
x6	x6	

Kinetic Law

Derived unit contains undeclared units

$$v_{11} = \mathrm{vol}\,(\mathrm{Cell}) \cdot \mathrm{k\_pB} \cdot [\mathrm{x5}] \quad (42)$$

9.12 Reaction r012___B_degradation

This is an irreversible reaction of one reactant forming no product.

Name r012 - B_degradation

Reaction equation

$$\mathrm{x6} \longrightarrow \emptyset \tag{43}$$

Reactant

Table 20: Properties of each reactant.

Id	Name	SBO
x6	x6	

Kinetic Law

Derived unit contains undeclared units

$$v_{12} = \mathrm{vol}\,(\mathrm{Cell}) \cdot \mathrm{d\_B} \cdot [\mathrm{x6}] \tag{44}$$

9.13 Reaction r013___mB_degradation

This is an irreversible reaction of one reactant forming no product.

Name r013 - mB_degradation

Reaction equation

$$\mathrm{x5} \longrightarrow \emptyset \tag{45}$$

Reactant

Table 21: Properties of each reactant.

Id	Name	SBO
x5	x5	

Kinetic Law

Derived unit contains undeclared units

$$v_{13} = \mathrm{vol}\,(\mathrm{Cell}) \cdot \mathrm{d\_mB} \cdot [\mathrm{x5}] \tag{46}$$

9.14 Reaction r014___mC_transcription

This is an irreversible reaction of no reactant forming one product influenced by two modifiers.

Name r014 - mC_transcription

Reaction equation

$$\emptyset \xrightarrow{\mathrm{x4,\ x6}} \mathrm{x7} \tag{47}$$

Modifiers

Table 22: Properties of each modifier.

Id	Name	SBO
x4	x4	
x6	x6	

Product

Table 23: Properties of each product.

Id	Name	SBO
x7	x7	

Kinetic Law

Derived unit contains undeclared units

$$v_{14} = \mathrm{vol}\,(\mathrm{Cell}) \cdot \mathrm{function\_for\_r014\_\_\_C\_translation}\,(\mathrm{k\_mC\_C\_gC}, [\mathrm{x4}], \mathrm{Beta\_1}, \mathrm{gamma\_4}, [\mathrm{x6}], \mathrm{Beta\_2}, \mathrm{gamma\_5}, \mathrm{gamma\_2}, \mathrm{gamma\_3}) \tag{48}$$

$$\begin{aligned}&\text{function\_for\_r014\_\_\_C\_translation}(\text{KmCCgC}, [\text{x4}], \text{Beta1},\\ &\quad \text{gamma4}, [\text{x6}], \text{Beta2}, \text{gamma5}, \text{gamma2}, \text{gamma3}) = \text{KmCCgC}\\ &\qquad \cdot \frac{[\text{x4}] + \text{Beta1} \cdot \text{gamma4} \cdot [\text{x6}] + \text{Beta2} \cdot \text{gamma5} \cdot [\text{x4}] \cdot [\text{x6}]}{\text{gamma2} + \text{gamma3} \cdot [\text{x4}] + \text{gamma4} \cdot [\text{x6}] + \text{gamma5} \cdot [\text{x4}] \cdot [\text{x6}]}\end{aligned} \tag{49}$$

$$\begin{aligned}&\text{function\_for\_r014\_\_\_C\_translation}(\text{KmCCgC}, [\text{x4}], \text{Beta1},\\ &\quad \text{gamma4}, [\text{x6}], \text{Beta2}, \text{gamma5}, \text{gamma2}, \text{gamma3}) = \text{KmCCgC}\\ &\qquad \cdot \frac{[\text{x4}] + \text{Beta1} \cdot \text{gamma4} \cdot [\text{x6}] + \text{Beta2} \cdot \text{gamma5} \cdot [\text{x4}] \cdot [\text{x6}]}{\text{gamma2} + \text{gamma3} \cdot [\text{x4}] + \text{gamma4} \cdot [\text{x6}] + \text{gamma5} \cdot [\text{x4}] \cdot [\text{x6}]}\end{aligned} \tag{50}$$

9.15 Reaction r015___C_translation

This is an irreversible reaction of one reactant forming two products.

Name r015 - C_translation

Reaction equation

$$\text{x7} \longrightarrow \text{x7} + \text{x8} \tag{51}$$

Reactant

Table 24: Properties of each reactant.

Id	Name	SBO
x7	x7	

Products

Table 25: Properties of each product.

Id	Name	SBO
x7	x7	
x8	x8	

Kinetic Law

Derived unit contains undeclared units

$$v_{15} = \text{vol}(\text{Cell}) \cdot \text{k\_pC} \cdot [\text{x7}] \tag{52}$$

9.16 Reaction r016___C_degradation

This is an irreversible reaction of one reactant forming no product.

Name r016 - C_degradation

Reaction equation

$$\mathrm{x8} \longrightarrow \emptyset \tag{53}$$

Reactant

Table 26: Properties of each reactant.

Id	Name	SBO
x8	x8	

Kinetic Law

Derived unit contains undeclared units

$$v_{16} = \mathrm{vol}\,(\mathrm{Cell}) \cdot \mathrm{d\_C} \cdot [\mathrm{x8}] \tag{54}$$

9.17 Reaction r017___mC_degradation

This is an irreversible reaction of one reactant forming no product.

Name r017 - mC_degradation

Reaction equation

$$\mathrm{x7} \longrightarrow \emptyset \tag{55}$$

Reactant

Table 27: Properties of each reactant.

Id	Name	SBO
x7	x7	

Kinetic Law

Derived unit contains undeclared units

$$v_{17} = \mathrm{vol}\,(\mathrm{Cell}) \cdot \mathrm{d\_mC} \cdot [\mathrm{x7}] \tag{56}$$

9.18 Reaction r018___AI2_dim_2

This is an irreversible reaction of one reactant forming no product.

Name r018 - AI2_dim_2

Reaction equation

$$\mathrm{x4} \longrightarrow \emptyset \tag{57}$$

Reactant

Table 28: Properties of each reactant.

Id	Name	SBO
x4	x4	

Kinetic Law

Derived unit contains undeclared units

$$v_{18} = \mathrm{vol}\,(\mathrm{Cell}) \cdot \mathrm{k\_3r} \cdot [\mathrm{x4}] \tag{58}$$

9.19 Reaction r019___AI2_dim_3

This is an irreversible reaction of no reactant forming two products.

Name r019 - AI2_dim_3

Reaction equation

$$\emptyset \longrightarrow \mathrm{x2} + \mathrm{x3} \tag{59}$$

Products

Table 29: Properties of each product.

Id	Name	SBO
x2	x2	
x3	x3	

Kinetic Law

Derived unit contains undeclared units

$$v_{19} = \mathrm{vol}\,(\mathrm{Cell}) \cdot \mathrm{function\_for\_r019\_\_\_AI2\_dim\_3}\,(\mathrm{k\_2r}, \mathrm{M}) \tag{60}$$

$$\mathrm{function\_for\_r019\_\_\_AI2\_dim\_3}\,(\mathrm{k\_2r}, \mathrm{M}) = \mathrm{k\_2r} \cdot \mathrm{M} \tag{61}$$

$$\mathrm{function\_for\_r019\_\_\_AI2\_dim\_3}\,(\mathrm{k\_2r}, \mathrm{M}) = \mathrm{k\_2r} \cdot \mathrm{M} \tag{62}$$

9.20 Reaction r020___AI2_dim_4

This is an irreversible reaction of no reactant forming one product.

Name r020 - AI2_dim_4

Reaction equation

$$\emptyset \longrightarrow \mathrm{x4} \tag{63}$$

Product

Table 30: Properties of each product.

Id	Name	SBO
x4	x4	

Kinetic Law

Derived unit contains undeclared units

$$v_{20} = \mathrm{vol}\,(\mathrm{Cell}) \cdot \mathrm{function\_for\_r020\_\_\_AI2\_dim\_4}\,(\mathrm{k\_3f}, \mathrm{M}) \tag{64}$$

$$\mathrm{function\_for\_r020\_\_\_AI2\_dim\_4}\,(\mathrm{k3}, \mathrm{M}) = \mathrm{k3} \cdot \mathrm{M} \cdot \mathrm{M} \tag{65}$$

$$\mathrm{function\_for\_r020\_\_\_AI2\_dim\_4}\,(\mathrm{k3}, \mathrm{M}) = \mathrm{k3} \cdot \mathrm{M} \cdot \mathrm{M} \tag{66}$$

9.21 Reaction r006b___I_transport

This is an irreversible reaction of one reactant forming two products.

Name r006b - I_transport

Reaction equation

$$\mathrm{x9} \longrightarrow \mathrm{x9} + \mathrm{x3} \tag{67}$$

Reactant

Table 31: Properties of each reactant.

Id	Name	SBO
x9	x9	

Products

Table 32: Properties of each product.

Id	Name	SBO
x9	x9	
x3	x3	

Kinetic Law

Derived unit contains undeclared units

$$v_{21} = \mathrm{k\_d} \cdot [\mathrm{x9}] \tag{68}$$

9.22 Reaction r006c___I_transport

This is an irreversible reaction of one reactant forming no product.

Name r006c - I_transport

Reaction equation

$$\mathrm{x9} \longrightarrow \emptyset \tag{69}$$

Reactant

Table 33: Properties of each reactant.

Id	Name	SBO
x9	x9	

Kinetic Law

Derived unit contains undeclared units

$$v_{22} = \text{vol}\,(\text{Extracellular}) \cdot \text{function\_for\_r006c}\,(\text{K\_cells}, \text{k\_d}, [\text{x9}]) \tag{70}$$

$$\text{function\_for\_r006c}\,(\text{Kcells}, \text{kd}, [\text{x9}]) = \text{Kcells} \cdot \text{kd} \cdot [\text{x9}] \tag{71}$$

$$\text{function\_for\_r006c}\,(\text{Kcells}, \text{kd}, [\text{x9}]) = \text{Kcells} \cdot \text{kd} \cdot [\text{x9}] \tag{72}$$

9.23 Reaction r006d___I_transport

This is an irreversible reaction of no reactant forming one product influenced by one modifier.

Name r006d - I_transport

Reaction equation

$$\emptyset \xrightarrow{\text{x3}} \text{x9} \tag{73}$$

Modifier

Table 34: Properties of each modifier.

Id	Name	SBO
x3	x3	

Product

Table 35: Properties of each product.

Id	Name	SBO
x9	x9	

Kinetic Law

Derived unit contains undeclared units

$$v_{23} = \text{function\_for\_r006d}(\text{K\_cells}, \text{k\_d}, [\text{x3}]) \tag{74}$$

$$\text{function\_for\_r006d}(\text{Kcells}, \text{kd}, [\text{x3}]) = \text{Kcells} \cdot \text{kd} \cdot [\text{x3}] \tag{75}$$

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 x1

Name x1

Notes `Original encoded model had simulation type set to 'fixed' and not 'reactions'`

Initial concentration $12.3973509933775\ \text{nmol} \cdot \mu\text{l}^{-1}$

Initial assignment `x1`

This species takes part in four reactions (as a reactant in `r002___A_translation`, `r003___mA_degradation` and as a product in `r001___mA_transcription`, `r002___A_translation`).

$$\frac{\text{d}}{\text{d}t}\text{x1} = v_1 + v_2 - v_2 - v_3 \tag{76}$$

10.2 Species x2

Name x2

Initial concentration $28336.8022705771\ \text{nmol} \cdot \mu\text{l}^{-1}$

Initial assignment `x2`

This species takes part in four reactions (as a reactant in `r004___A_degradation`, `r005___AI2_dim_1` and as a product in `r002___A_translation`, `r019___AI2_dim_3`).

$$\frac{\text{d}}{\text{d}t}\text{x2} = v_2 + v_{19} - v_4 - v_5 \tag{77}$$

10.3 Species x3

Name x3

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

This species takes part in six reactions (as a reactant in r005___AI2_dim_1, r006a___I_transport, r007___I_degradation and as a product in r019___AI2_dim_3, r006b___I_transport and as a modifier in r006d___I_transport).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{x3} = v_{19} + v_{21} - v_5 - v_6 - v_7 \tag{78}$$

10.4 Species x4

Name x4

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

This species takes part in five reactions (as a reactant in r009___AI2_degradation, r018___AI2_dim_2 and as a product in r020___AI2_dim_4 and as a modifier in r010___mB_transcription, r014___mC_transcription).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{x4} = v_{20} - v_9 - v_{18} \tag{79}$$

10.5 Species x5

Name x5

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

This species takes part in four reactions (as a reactant in r011___B_translation, r013___mB_degradation and as a product in r010___mB_transcription, r011___B_translation).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{x5} = v_{10} + v_{11} - v_{11} - v_{13} \tag{80}$$

10.6 Species x6

Name x6

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

This species takes part in three reactions (as a reactant in r012___B_degradation and as a product in r011___B_translation and as a modifier in r014___mC_transcription).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{x6} = v_{11} - v_{12} \tag{81}$$

10.7 Species x7

Name x7

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

This species takes part in four reactions (as a reactant in r015___C_translation, r017___mC_degradation and as a product in r014___mC_transcription, r015___C_translation).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{x7} = v_{14} + v_{15} - v_{15} - v_{17} \tag{82}$$

10.8 Species x8

Name x8

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

This species takes part in two reactions (as a reactant in r016___C_degradation and as a product in r015___C_translation).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{x8} = v_{15} - v_{16} \tag{83}$$

10.9 Species x9

Name x9

Initial concentration $9000\ \mathrm{nmol} \cdot \mu\mathrm{l}^{-1}$

Initial assignment x9

This species takes part in five reactions (as a reactant in r008___Ie_degradation, r006b___I_transport, r006c___I_transport and as a product in r006b___I_transport, r006d___I_transport).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{x9} = v_{21} + v_{23} - v_{8} - v_{21} - v_{22} \tag{84}$$

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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