SBML Model Report

Model name: “Karapetyan2016 - Genetic oscillatory network - Repressor Titration Circuit (RTC)”

May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by the following three authors: Nick Juty[1], Vijayalakshmi Chelliah[2] and Sargis Karapetyan[3] at January 26th 2015 at 5:46 p. m. and last time modified at March 17th 2016 at 1:18 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	23	function definitions	1
global parameters	25	unit definitions	3
rules	9	initial assignments	6

Model Notes

Karapetyan2016 - Genetic oscillatory network - Repressor Titration Circuit (RTC)

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This model is described in the article:Role of DNA binding sites and slow unbinding kinetics in titration-based oscillators. Karapetyan S, Buchler NE. Phys Rev E Stat Nonlin Soft Matter Phys 2015 Dec; 92(6-1): 062712

Abstract:

Genetic oscillators, such as circadian clocks, are constantly perturbed by molecular noise arising from the small number of molecules involved in gene regulation. One of the strongest sources of stochasticity is the binary noise that arises from the binding of a regulatory protein to a promoter in the chromosomal DNA. In this study, we focus on two minimal oscillators based on activator titration and repressor titration to understand the key parameters that are important for oscillations and for overcoming binary noise. We show that the rate of unbinding from the DNA, despite traditionally being considered a fast parameter, needs to be slow to broaden the space of oscillatory solutions. The addition of multiple, independent DNA binding sites further expands the oscillatory parameter space for the repressor-titration oscillator and lengthens the period of both oscillators. This effect is a combination of increased effective delay of the unbinding kinetics due to multiple binding sites and increased promoter ultrasensitivity that is specific for repression. We then use stochastic simulation to show that multiple binding sites increase the coherence of oscillations by mitigating the binary noise. Slow values of DNA unbinding rate are also effective in alleviating molecular noise due to the increased distance from the bifurcation point. Our work demonstrates how the number of DNA binding sites and slow unbinding kinetics, which are often omitted in biophysical models of gene circuits, can have a significant impact on the temporal and stochastic dynamics of genetic oscillators.

This model is hosted on BioModels Database and identified by: BIOMD0000000587.

To cite BioModels Database, please use: BioModels Database: An enhanced, curated and annotated resource for published quantitative kinetic models.

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 `volume`

Name volume

Definition dimensionless

2.2 Unit `time`

Name time

Definition 60 s

2.3 Unit substance

Name substance

Definition item

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
yeast	yeast	0000290	3	1	dimensionless	☑	

3.1 Compartment yeast

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

Name yeast

SBO:0000290 physical compartment

4 Species

This model contains ten 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
G0	G0	yeast	item $\cdot$ dimensionless^{-1}	⊟	⊟
G1	G1	yeast	item $\cdot$ dimensionless^{-1}	⊟	⊟
rR	rR	yeast	item $\cdot$ dimensionless^{-1}	⊟	⊟
I	I	yeast	item $\cdot$ dimensionless^{-1}	⊟	⊟
rI	rI	yeast	item $\cdot$ dimensionless^{-1}	⊟	⊟
R	R	yeast	item $\cdot$ dimensionless^{-1}	⊟	⊟
RI	RI	yeast	item $\cdot$ dimensionless^{-1}	⊟	⊟
R2	R2	yeast	item $\cdot$ dimensionless^{-1}	⊟	⊟
G2	G2	yeast	item $\cdot$ dimensionless^{-1}	⊟	⊟
G3	G3	yeast	item $\cdot$ dimensionless^{-1}	⊟	⊟

5 Parameters

This model contains 25 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Theta	Theta	0000338	0.020		☑
Alpha	Alpha		$2.49202551834131 \cdot 10^{-4}$		☐
rho_f	rho_f		0.893		☑
rho_b	rho_b		0.246		☐
rho_0	rho_0		0.469		☐
beta	beta		14.109		☑
delta_m	delta_m		0.016		☑
delta_p	delta_p		0.008		☑
gamma	gamma		0.025		☑
epsilon	epsilon		0.024		☑
epsilon_1	epsilon_1		6.000		☑
a_01	a_01		$2.49202551834131 \cdot 10^{-4}$		☐
a_12	a_12		0.000		☐
a_23	a_23		0.000		☐
t_10	t_10		0.020		☐
t_21	t_21		0.000		☐
t_32	t_32		0.000		☐
_3sites	3sites		0.000		☑
f	f		3.630		☑
ModelValue_17	Initial for 3sites		0.000		☑
ModelValue_1	Initial for Alpha		$2.49202551834131 \cdot 10^{-4}$		☑
ModelValue_0	Initial for Theta		0.020		☑
ModelValue_18	Initial for f		3.630		☑
ModelValue_3	Initial for rho_b		0.246		☑
ModelValue_2	Initial for rho_f		0.893		☑

6 Initialassignments

This is an overview of six initialassignments.

6.1 Initialassignment ModelValue_17

Derived unit contains undeclared units

Math _3sites

6.2 Initialassignment ModelValue_1

Derived unit contains undeclared units

Math Alpha

6.3 Initialassignment ModelValue_0

Derived unit contains undeclared units

Math Theta

6.4 Initialassignment ModelValue_18

Derived unit contains undeclared units

Math f

6.5 Initialassignment ModelValue_3

Derived unit contains undeclared units

Math rho_b

6.6 Initialassignment ModelValue_2

Derived unit contains undeclared units

Math rho_f

7 Function definition

This is an overview of one function definition.

7.1 Function definition Constant_flux__irreversible

Name Constant flux (irreversible)

Argument v

Mathematical Expression

$$v \tag{1}$$

8 Rules

This is an overview of nine rules.

8.1 Rule `Alpha`

Rule `Alpha` is an assignment rule for parameter `Alpha`:

$$\text{Alpha} = \frac{\text{ModelValue\_0}}{24 \cdot 3.344} \tag{2}$$

8.2 Rule `rho_b`

Rule `rho_b` is an assignment rule for parameter `rho_b`:

$$\text{rho\_b} = \frac{\text{ModelValue\_2}}{\text{ModelValue\_18}} \tag{3}$$

8.3 Rule `rho_0`

Rule `rho_0` is an assignment rule for parameter `rho_0`:

$$\text{rho\_0} = \sqrt{2} \tag{4}$$

8.4 Rule `a_01`

Rule `a_01` is an assignment rule for parameter `a_01`:

$$\text{a\_01} = \begin{cases} 3 \cdot \text{ModelValue\_1} & \text{if ModelValue\_17} = 1 \\ \text{ModelValue\_1} & \text{otherwise} \end{cases} \tag{5}$$

8.5 Rule `a_12`

Rule `a_12` is an assignment rule for parameter `a_12`:

$$\text{a\_12} = \begin{cases} 2 \cdot \text{ModelValue\_1} & \text{if ModelValue\_17} = 1 \\ 0 & \text{otherwise} \end{cases} \tag{6}$$

8.6 Rule `a_23`

Rule `a_23` is an assignment rule for parameter `a_23`:

$$\text{a\_23} = \begin{cases} 1 \cdot \text{ModelValue\_1} & \text{if ModelValue\_17} = 1 \\ 0 & \text{otherwise} \end{cases} \tag{7}$$

8.7 Rule t_10

Rule t_10 is an assignment rule for parameter t_10:

$$\mathrm{t\_10} = \mathrm{ModelValue\_0} \tag{8}$$

8.8 Rule t_21

Rule t_21 is an assignment rule for parameter t_21:

$$\mathrm{t\_21} = \begin{cases} 2 \cdot \mathrm{ModelValue\_0} & \text{if } \mathrm{ModelValue\_17} = 1 \\ 0 & \text{otherwise} \end{cases} \tag{9}$$

8.9 Rule t_32

Rule t_32 is an assignment rule for parameter t_32:

$$\mathrm{t\_32} = \begin{cases} 3 \cdot \mathrm{ModelValue\_0} & \text{if } \mathrm{ModelValue\_17} = 1 \\ 0 & \text{otherwise} \end{cases} \tag{10}$$

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	G1___G0__R2	G1 -> G0 + R2	$G1 \xrightarrow{G1} G0 + R2$	
2	G0__R2___G1	G0 + R2 -> G1	$G0 + R2 \xrightarrow{G0,\ R2} G1$	
3	G0___G0__rR	G0 -> G0 + rR	$G0 \xrightarrow{G0} G0 + rR$	
4	G1___G1__rR	G1 -> G1 + rR	$G1 \xrightarrow{G1} G1 + rR$	
5	rR___	rR ->	$rR \xrightarrow{rR} \emptyset$	
6	___rI	-> rI	$\emptyset \longrightarrow rI$	
7	rI___	rI ->	$rI \xrightarrow{rI} \emptyset$	
8	rR___rR__R	rR -> rR + R	$rR \xrightarrow{rR} rR + R$	
9	I___	I ->	$I \xrightarrow{I} \emptyset$	
10	rI___rI__I	rI -> rI + I	$rI \xrightarrow{rI} rI + I$	
11	R___	R ->	$R \xrightarrow{R} \emptyset$	
12	R__I___RI	R + I -> RI	$R + I \xrightarrow{R,\ I} RI$	
13	_2__R___R2	2 * R -> R2	$2\,R \xrightarrow{R} R2$	
14	R2___2__R	R2 -> 2 * R	$R2 \xrightarrow{R2} 2\,R$	
15	RI___R__I	RI -> R + I	$RI \xrightarrow{RI} R + I$	
16	RI___	RI ->	$RI \xrightarrow{RI} \emptyset$	
17	R2___	R2 ->	$R2 \xrightarrow{R2} \emptyset$	

№	Id	Name	Reaction Equation	SBO
18	G1___R2____G2	G1 + R2 -> G2	$\mathrm{G1} + \mathrm{R2} \xrightarrow{\mathrm{G1,\ R2}} \mathrm{G2}$	
19	G2____G1___R2	G2 -> G1 + R2	$\mathrm{G2} \xrightarrow{\mathrm{G2}} \mathrm{G1} + \mathrm{R2}$	
20	G2____G2___rR	G2 -> G2 + rR	$\mathrm{G2} \xrightarrow{\mathrm{G2}} \mathrm{G2} + \mathrm{rR}$	
21	G2___R2____G3	G2 + R2 -> G3	$\mathrm{G2} + \mathrm{R2} \xrightarrow{\mathrm{G2,\ R2}} \mathrm{G3}$	
22	G3____G2___R2	G3 -> G2 + R2	$\mathrm{G3} \xrightarrow{\mathrm{G3}} \mathrm{G2} + \mathrm{R2}$	
23	G3____G3___rR	G3 -> G3 + rR	$\mathrm{G3} \xrightarrow{\mathrm{G3}} \mathrm{G3} + \mathrm{rR}$	

9.1 Reaction G1___G0__R2

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

Name G1 -> G0 + R2

Reaction equation

$$\mathrm{G1} \xrightarrow{\mathrm{G1}} \mathrm{G0} + \mathrm{R2} \tag{11}$$

Reactant

Table 6: Properties of each reactant.

Id	Name	SBO
G1	G1	

Modifier

Table 7: Properties of each modifier.

Id	Name	SBO
G1	G1	

Products

Table 8: Properties of each product.

Id	Name	SBO
G0	G0	
R2	R2	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \mathrm{vol}\,(\mathrm{yeast}) \cdot \mathrm{t\_10} \cdot [\mathrm{G1}] \tag{12}$$

9.2 Reaction G0__R2___G1

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

Name G0 + R2 -> G1

Reaction equation

$$\mathrm{G0} + \mathrm{R2} \xrightarrow{\mathrm{G0,\ R2}} \mathrm{G1} \tag{13}$$

Reactants

Table 9: Properties of each reactant.

Id	Name	SBO
G0	G0	
R2	R2	

Modifiers

Table 10: Properties of each modifier.

Id	Name	SBO
G0	G0	
R2	R2	

Product

Table 11: Properties of each product.

Id	Name	SBO
G1	G1	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \mathrm{vol}\,(\mathrm{yeast}) \cdot \mathrm{a\_01} \cdot [\mathrm{G0}] \cdot [\mathrm{R2}] \tag{14}$$

9.3 Reaction G0___G0__rR

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

Name G0 -> G0 + rR

Reaction equation

$$\mathrm{G0} \xrightarrow{\mathrm{G0}} \mathrm{G0} + \mathrm{rR} \tag{15}$$

Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
G0	G0	

Modifier

Table 13: Properties of each modifier.

Id	Name	SBO
G0	G0	

Products

Table 14: Properties of each product.

Id	Name	SBO
G0	G0	
rR	rR	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \mathrm{vol}\,(\mathrm{yeast}) \cdot \mathrm{rho\_f} \cdot [\mathrm{G0}] \tag{16}$$

9.4 Reaction G1___G1___rR

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

Name G1 -> G1 + rR

Reaction equation

$$\mathrm{G1} \xrightarrow{\mathrm{G1}} \mathrm{G1} + \mathrm{rR} \tag{17}$$

Reactant

Table 15: Properties of each reactant.

Id	Name	SBO
G1	G1	

Modifier

Table 16: Properties of each modifier.

Id	Name	SBO
G1	G1	

Products

Table 17: Properties of each product.

Id	Name	SBO
G1	G1	
rR	rR	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \mathrm{vol}\,(\mathrm{yeast}) \cdot \mathrm{rho\_b} \cdot [\mathrm{G1}] \tag{18}$$

9.5 Reaction rR___

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

Name rR ->

Reaction equation

$$\mathrm{rR} \xrightarrow{\mathrm{rR}} \emptyset \tag{19}$$

Reactant

Table 18: Properties of each reactant.

Id	Name	SBO
rR	rR	

Modifier

Table 19: Properties of each modifier.

Id	Name	SBO
rR	rR	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \mathrm{vol}\left(\mathrm{yeast}\right) \cdot \mathrm{delta\_m} \cdot \left[\mathrm{rR}\right] \tag{20}$$

9.6 Reaction ____rI

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

Name -> rI

Reaction equation

$$\emptyset \longrightarrow \mathrm{rI} \tag{21}$$

Product

Table 20: Properties of each product.

Id	Name	SBO
rI	rI	

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \mathrm{vol}\left(\mathrm{yeast}\right) \cdot \mathrm{Constant\_flux\_\_irreversible}\left(\mathrm{rho\_0}\right) \tag{22}$$

$$\mathrm{Constant\_flux\_\_irreversible}\left(\mathrm{v}\right) = \mathrm{v} \tag{23}$$

$$\mathrm{Constant\_flux\_\_irreversible}\left(\mathrm{v}\right) = \mathrm{v} \tag{24}$$

9.7 Reaction rI___

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

Name rI ->

Reaction equation

$$\mathrm{rI} \xrightarrow{\mathrm{rI}} \emptyset \tag{25}$$

Reactant

Table 21: Properties of each reactant.

Id	Name	SBO
rI	rI	

Modifier

Table 22: Properties of each modifier.

Id	Name	SBO
rI	rI	

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \mathrm{vol}\,(\mathrm{yeast}) \cdot \mathrm{delta\_m} \cdot [\mathrm{rI}] \tag{26}$$

9.8 Reaction rR____rR___R

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

Name rR -> rR + R

Reaction equation

$$\mathrm{rR} \xrightarrow{\mathrm{rR}} \mathrm{rR} + \mathrm{R} \tag{27}$$

Reactant

Table 23: Properties of each reactant.

Id	Name	SBO
rR	rR	

Modifier

Table 24: Properties of each modifier.

Id	Name	SBO
rR	rR	

Products

Table 25: Properties of each product.

Id	Name	SBO
rR	rR	
R	R	

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \mathrm{vol}\,(\mathrm{yeast}) \cdot \mathrm{beta} \cdot [\mathrm{rR}] \tag{28}$$

9.9 Reaction I___

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

Name I ->

Reaction equation

$$\mathrm{I} \xrightarrow{\mathrm{I}} \emptyset \tag{29}$$

Reactant

Table 26: Properties of each reactant.

Id	Name	SBO
I	I	

Modifier

Table 27: Properties of each modifier.

Id	Name	SBO
I	I	

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \mathrm{vol}\,(\mathrm{yeast}) \cdot \mathrm{delta\_p} \cdot [\mathrm{I}] \tag{30}$$

9.10 Reaction rI____rI___I

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

Name rI -> rI + I

Reaction equation

$$\mathrm{rI} \xrightarrow{\mathrm{rI}} \mathrm{rI} + \mathrm{I} \tag{31}$$

Reactant

Table 28: Properties of each reactant.

Id	Name	SBO
rI	rI	

Modifier

Table 29: Properties of each modifier.

Id	Name	SBO
rI	rI	

Products

Table 30: Properties of each product.

Id	Name	SBO
rI	rI	
I	I	

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = \mathrm{vol}\,(\mathrm{yeast}) \cdot \mathrm{beta} \cdot [\mathrm{rI}] \tag{32}$$

9.11 Reaction R___

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

Name R ->

Reaction equation

$$\mathrm{R} \xrightarrow{\mathrm{R}} \emptyset \tag{33}$$

Reactant

Table 31: Properties of each reactant.

Id	Name	SBO
R	R	

Modifier

Table 32: Properties of each modifier.

Id	Name	SBO
R	R	

Kinetic Law

Derived unit contains undeclared units

$$v_{11} = \mathrm{vol}\,(\mathrm{yeast}) \cdot \mathrm{delta\_p} \cdot [\mathrm{R}] \tag{34}$$

9.12 Reaction R___I____RI

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

Name R + I -> RI

Reaction equation

$$\mathrm{R} + \mathrm{I} \xrightarrow{\mathrm{R,\ I}} \mathrm{RI} \tag{35}$$

Reactants

Table 33: Properties of each reactant.

Id	Name	SBO
R	R	
I	I	

Modifiers

Table 34: Properties of each modifier.

Id	Name	SBO
R	R	
I	I	

Product

Table 35: Properties of each product.

Id	Name	SBO
RI	RI	

Kinetic Law

Derived unit contains undeclared units

$$v_{12} = \mathrm{vol}\,(\mathrm{yeast}) \cdot \mathrm{gamma} \cdot [\mathrm{R}] \cdot [\mathrm{I}] \tag{36}$$

9.13 Reaction _2___R____R2

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

Name 2 * R -> R2

Reaction equation

$$2\,\mathrm{R} \xrightarrow{\mathrm{R}} \mathrm{R2} \tag{37}$$

Reactant

Table 36: Properties of each reactant.

Id	Name	SBO
R	R	

Modifier

Table 37: Properties of each modifier.

Id	Name	SBO
R	R	

Product

Table 38: Properties of each product.

Id	Name	SBO
R2	R2	

Kinetic Law

Derived unit contains undeclared units

$$v_{13} = \mathrm{vol}\,(\mathrm{yeast}) \cdot \mathrm{gamma} \cdot [\mathrm{R}]^2 \tag{38}$$

9.14 Reaction R2____2___R

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

Name R2 -> 2 * R

Reaction equation

$$\mathrm{R2} \xrightarrow{\mathrm{R2}} 2\,\mathrm{R} \tag{39}$$

Reactant

Table 39: Properties of each reactant.

Id	Name	SBO
R2	R2	

Modifier

Table 40: Properties of each modifier.

Id	Name	SBO
R2	R2	

Product

Table 41: Properties of each product.

Id	Name	SBO
R	R	

Kinetic Law

Derived unit contains undeclared units

$$v_{14} = \mathrm{vol}\,(\mathrm{yeast}) \cdot \mathrm{epsilon\_1} \cdot [\mathrm{R2}] \tag{40}$$

9.15 Reaction RI___R__I

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

Name RI -> R + I

Reaction equation

$$\mathrm{RI} \xrightarrow{\mathrm{RI}} \mathrm{R} + \mathrm{I} \tag{41}$$

Reactant

Table 42: Properties of each reactant.

Id	Name	SBO
RI	RI	

Modifier

Table 43: Properties of each modifier.

Id	Name	SBO
RI	RI	

Products

Table 44: Properties of each product.

Id	Name	SBO
R	R	
I	I	

Kinetic Law

Derived unit contains undeclared units

$$v_{15} = \mathrm{vol}\,(\mathrm{yeast}) \cdot \mathrm{epsilon} \cdot [\mathrm{RI}] \tag{42}$$

9.16 Reaction RI___

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

Name RI ->

Reaction equation

$$\mathrm{RI} \xrightarrow{\mathrm{RI}} \emptyset \tag{43}$$

Reactant

Table 45: Properties of each reactant.

Id	Name	SBO
RI	RI	

Modifier

Table 46: Properties of each modifier.

Id	Name	SBO
RI	RI	

Kinetic Law

Derived unit contains undeclared units

$$v_{16} = \mathrm{vol}\,(\mathrm{yeast}) \cdot \mathrm{delta\_p} \cdot [\mathrm{RI}] \tag{44}$$

9.17 Reaction R2___

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

Name R2 ->

Reaction equation

$$\mathrm{R2} \xrightarrow{\mathrm{R2}} \emptyset \tag{45}$$

Reactant

Table 47: Properties of each reactant.

Id	Name	SBO
R2	R2	

Modifier

Table 48: Properties of each modifier.

Id	Name	SBO
R2	R2	

Kinetic Law

Derived unit contains undeclared units

$$v_{17} = \mathrm{vol}\,(\mathrm{yeast}) \cdot \mathrm{delta\_p} \cdot [\mathrm{R2}] \tag{46}$$

9.18 Reaction G1__R2____G2

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

Name G1 + R2 -> G2

Reaction equation

$$\mathrm{G1} + \mathrm{R2} \xrightarrow{\mathrm{G1,\ R2}} \mathrm{G2} \tag{47}$$

Reactants

Table 49: Properties of each reactant.

Id	Name	SBO
G1	G1	
R2	R2	

Modifiers

Table 50: Properties of each modifier.

Id	Name	SBO
G1	G1	
R2	R2	

Product

Table 51: Properties of each product.

Id	Name	SBO
G2	G2	

Kinetic Law

Derived unit contains undeclared units

$$v_{18} = \mathrm{vol}\,(\mathrm{yeast}) \cdot \mathrm{a\_12} \cdot [\mathrm{G1}] \cdot [\mathrm{R2}] \tag{48}$$

9.19 Reaction G2____G1___R2

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

Name G2 -> G1 + R2

Reaction equation

$$\mathrm{G2} \xrightarrow{\mathrm{G2}} \mathrm{G1} + \mathrm{R2} \tag{49}$$

Reactant

Table 52: Properties of each reactant.

Id	Name	SBO
G2	G2	

Modifier

Table 53: Properties of each modifier.

Id	Name	SBO
G2	G2	

Products

Table 54: Properties of each product.

Id	Name	SBO
G1	G1	
R2	R2	

Kinetic Law

Derived unit contains undeclared units

$$v_{19} = \mathrm{vol}\,(\mathrm{yeast}) \cdot \mathrm{t\_21} \cdot [\mathrm{G2}] \tag{50}$$

9.20 Reaction G2____G2___rR

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

Name G2 -> G2 + rR

Reaction equation

$$\mathrm{G2} \xrightarrow{\mathrm{G2}} \mathrm{G2} + \mathrm{rR} \tag{51}$$

Reactant

Table 55: Properties of each reactant.

Id	Name	SBO
G2	G2	

Modifier

Table 56: Properties of each modifier.

Id	Name	SBO
G2	G2	

Products

Table 57: Properties of each product.

Id	Name	SBO
G2	G2	
rR	rR	

Kinetic Law

Derived unit contains undeclared units

$$v_{20} = \mathrm{vol}\,(\mathrm{yeast}) \cdot \mathrm{rho\_b} \cdot [\mathrm{G2}] \tag{52}$$

9.21 Reaction G2___R2____G3

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

Name G2 + R2 -> G3

Reaction equation

$$\mathrm{G2} + \mathrm{R2} \xrightarrow{\mathrm{G2,\ R2}} \mathrm{G3} \tag{53}$$

Reactants

Table 58: Properties of each reactant.

Id	Name	SBO
G2	G2	
R2	R2	

Modifiers

Table 59: Properties of each modifier.

Id	Name	SBO
G2	G2	
R2	R2	

Product

Table 60: Properties of each product.

Id	Name	SBO
G3	G3	

Kinetic Law

Derived unit contains undeclared units

$$v_{21} = \mathrm{vol}\,(\mathrm{yeast}) \cdot \mathrm{a\_23} \cdot [\mathrm{G2}] \cdot [\mathrm{R2}] \tag{54}$$

9.22 Reaction G3____G2___R2

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

Name G3 -> G2 + R2

Reaction equation

$$\mathrm{G3} \xrightarrow{\mathrm{G3}} \mathrm{G2} + \mathrm{R2} \tag{55}$$

Reactant

Table 61: Properties of each reactant.

Id	Name	SBO
G3	G3	

Modifier

Table 62: Properties of each modifier.

Id	Name	SBO
G3	G3	

Products

Table 63: Properties of each product.

Id	Name	SBO
G2	G2	
R2	R2	

Kinetic Law

Derived unit contains undeclared units

$$v_{22} = \mathrm{vol}\,(\mathrm{yeast}) \cdot \mathrm{t\_32} \cdot [\mathrm{G3}] \tag{56}$$

9.23 Reaction G3___G3__rR

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

Name G3 -> G3 + rR

Reaction equation

$$\mathrm{G3} \xrightarrow{\mathrm{G3}} \mathrm{G3} + \mathrm{rR} \tag{57}$$

Reactant

Table 64: Properties of each reactant.

Id	Name	SBO
G3	G3	

Modifier

Table 65: Properties of each modifier.

Id	Name	SBO
G3	G3	

Products

Table 66: Properties of each product.

Id	Name	SBO
G3	G3	
rR	rR	

Kinetic Law

Derived unit contains undeclared units

$$v_{23} = \mathrm{vol}\,(\mathrm{yeast}) \cdot \mathrm{rho\_b} \cdot [\mathrm{G3}] \tag{58}$$

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 G0

Name G0

SBO:0000196 concentration of an entity pool

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

This species takes part in six reactions (as a reactant in G0__R2____G1, G0____G0__rR and as a product in G1____G0__R2, G0____G0__rR and as a modifier in G0__R2____G1, G0____G0__rR).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{G0} = v_1 + v_3 - v_2 - v_3 \tag{59}$$

10.2 Species G1

Name G1

SBO:0000196 concentration of an entity pool

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

This species takes part in nine reactions (as a reactant in G1____G0__R2, G1____G1__rR, G1__R2____G2 and as a product in G0__R2____G1, G1____G1__rR, G2____G1__R2 and as a modifier in G1____G0__R2, G1____G1__rR, G1__R2____G2).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{G1} = v_2 + v_4 + v_{19} - v_1 - v_4 - v_{18} \tag{60}$$

10.3 Species rR

Name rR

SBO:0000278 messenger RNA

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

This species takes part in nine reactions (as a reactant in rR___, rR____rR__R and as a product in G0____G0__rR, G1____G1__rR, rR____rR__R, G2____G2__rR, G3____G3__rR and as a modifier in rR___, rR____rR__R).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{rR} = v_3 + v_4 + v_8 + v_{20} + v_{23} - v_5 - v_8 \tag{61}$$

10.4 Species I

Name I

SBO:0000020 inhibitor

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

This species takes part in six reactions (as a reactant in I___, R__I____RI and as a product in rI____rI__I, RI____R__I and as a modifier in I___, R__I____RI).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{I} = v_{10} + v_{15} - v_9 - v_{12} \tag{62}$$

10.5 Species rI

Name rI

SBO:0000278 messenger RNA

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

This species takes part in six reactions (as a reactant in rI___, rI____rI___I and as a product in ____rI, rI____rI___I and as a modifier in rI___, rI____rI___I).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{rI} = v_6 + v_{10} - v_7 - v_{10} \tag{63}$$

10.6 Species R

Name R

SBO:0000207 non-competitive inhibitor

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

This species takes part in nine reactions (as a reactant in R___, R___I____RI, _2___R____R2 and as a product in rR____rR___R, R2____2___R, RI____R___I and as a modifier in R___, R___I____RI, _2___R____R2).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{R} = v_8 + 2\,v_{14} + v_{15} - v_{11} - v_{12} - 2\,v_{13} \tag{64}$$

10.7 Species RI

Name RI

SBO:0000609 heterodimer

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

This species takes part in five reactions (as a reactant in RI____R___I, RI___ and as a product in R___I____RI and as a modifier in RI____R___I, RI___).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{RI} = v_{12} - v_{15} - v_{16} \tag{65}$$

10.8 Species R2

Name R2

SBO:0000608 homodimer

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

This species takes part in 14 reactions (as a reactant in G0___R2___G1, R2___2___R, R2___, G1-___R2___G2, G2___R2___G3 and as a product in G1___G0___R2, _2___R___R2, G2___G1___R2, G3___G2___R2 and as a modifier in G0___R2___G1, R2___2___R, R2___, G1___R2___G2, G2___R2-___G3).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{R2} = v_1 + v_{13} + v_{19} + v_{22} - v_2 - v_{14} - v_{17} - v_{18} - v_{21} \tag{66}$$

10.9 Species G2

Name G2

SBO:0000196 concentration of an entity pool

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

This species takes part in nine reactions (as a reactant in G2___G1___R2, G2___G2___rR, G2__-_R2___G3 and as a product in G1___R2___G2, G2___G2___rR, G3___G2___R2 and as a modifier in G2___G1___R2, G2___G2___rR, G2___R2___G3).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{G2} = v_{18} + v_{20} + v_{22} - v_{19} - v_{20} - v_{21} \tag{67}$$

10.10 Species G3

Name G3

SBO:0000196 concentration of an entity pool

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

This species takes part in six reactions (as a reactant in G3___G2___R2, G3___G3___rR and as a product in G2___R2___G3, G3___G3___rR and as a modifier in G3___G2___R2, G3___G3___rR).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{G3} = v_{21} + v_{23} - v_{22} - v_{23} \tag{68}$$

A Glossary of Systems Biology Ontology Terms

SBO:0000020 inhibitor: Substance that decreases the probability of a chemical reaction without itself being consumed or transformed by the reaction

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

SBO:0000207 non-competitive inhibitor: Substance that decreases the probability of a chemical reaction, without itself being consumed or transformed by the reaction, and without sterically hindering the interaction between reactants.

SBO:0000278 messenger RNA: A messenger RNA is a ribonucleic acid synthesized during the transcription of a gene, and that carries the information to encode one or several proteins

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:0000338 dissociation rate constant: Rate with which a complex dissociates into its components

SBO:0000608 homodimer: A macromolecular complex composed of precisely two identical monomeric units, which are usually non-covalently bound

SBO:0000609 heterodimer: A macromolecular complex composed of precisely two non-identical monomeric units, which are usually non-covalently bound

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