SBML Model Report

Model name: "Karapetyan2016 - Genetic oscillatory network - Activator Titration Circuit (ATC)"



May 5, 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 - Activator Titration Circuit (ATC)

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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: BIOMD0000000586.

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

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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 m²

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	Ø	

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 Condi- tion
GO	G0	yeast	item · ⊟ dimensionless ⁻¹	
G1	G1	yeast	item \cdot \square dimensionless ⁻¹	
rA	rA	yeast	item \Box dimensionless ⁻¹	\Box
I	I	yeast	item $\cdot \Box$ dimensionless ⁻¹	
rI	rI	yeast	item $\cdot \Box$ dimensionless ⁻¹	
A	A	yeast	item $\cdot \Box$ dimensionless ⁻¹	
AI	AI	yeast	item $\cdot \Box$ dimensionless ⁻¹	
A2	A2	yeast	item \cdot \boxminus dimensionless ⁻¹	
G2	G2	yeast	item $\cdot \Box$ dimensionless ⁻¹	
G3	G3	yeast	item \cdot \square dimensionless ⁻¹	

5 Parameters

This model contains 25 global parameters.

Table 4: Properties of each parameter.

			s of each parameter		
Id	Name	SBO	Value	Unit	Constant
Theta	Theta	0000338	0.020		Ø
Alpha	Alpha	2.4	9202551834131 · 1	0^{-4}	
${\tt rho_f}$	rho_f		0.178		
rho_b	rho_b		5.343		
${\tt rho_0}$	rho_0		0.975		\Box
beta	beta		14.109		
delta_m	delta_m		0.019		
delta_p	delta_p		0.008		
gamma	gamma		0.025		
epsilon	epsilon		0.024		
$epsilon_1$	epsilon_1		6.000		
a_01	a_01	2.4	9202551834131 · 1	0^{-4}	
a_12	$a_{-}12$		0.000		
a_23	a_23		0.000		
t10	$t_{-}10$		0.020		
t_21	t_21		0.000		
t_32	t_32		0.000		
$_3\mathtt{sites}$	3sites		0.000		
f	f		30.000		
ModelValue-	Initial for 3sites		0.000		
_17					
${\tt ModelValue_1}$	Initial for Alpha	2.4	9202551834131 · 1	0^{-4}	
$ModelValue_0$	Initial for Theta		0.020		
ModelValue-	Initial for f		30.000		
_18					
$ModelValue_3$	Initial for rho_b		5.343		\square
${\tt ModelValue_2}$	Initial for rho_f		0.178		

6 Initialassignments

This is an overview of six initial assignments.

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 (1)

8 Rules

This is an overview of nine rules.

8.1 Rule Alpha

Rule Alpha is an assignment rule for parameter Alpha:

$$Alpha = \frac{ModelValue_0}{24 \cdot 3.344}$$
 (2)

8.2 Rule rho_b

Rule rho_b is an assignment rule for parameter rho_b:

$$rho_b = ModelValue_2 \cdot ModelValue_18$$
 (3)

8.3 Rule rho_0

Rule rho_0 is an assignment rule for parameter rho_0:

$$rho_{-}0 = \sqrt{2} \tag{4}$$

8.4 Rule a_01

Rule a_01 is an assignment rule for parameter a_01:

$$a_01 = \begin{cases} 3 \cdot ModelValue_1 & \text{if ModelValue}_17 = 1\\ ModelValue_1 & \text{otherwise} \end{cases}$$
 (5)

8.5 Rule a_12

Rule a_12 is an assignment rule for parameter a_12:

$$a_{-}12 = \begin{cases} 2 \cdot ModelValue_{-}1 & \text{if ModelValue}_{-}17 = 1\\ 0 & \text{otherwise} \end{cases}$$
 (6)

8.6 Rule a_23

Rule a_23 is an assignment rule for parameter a_23:

$$a_{-}23 = \begin{cases} 1 \cdot ModelValue_{-}1 & \text{if ModelValue}_{-}17 = 1\\ 0 & \text{otherwise} \end{cases}$$
 (7)

8.7 Rule t_10

Rule t_10 is an assignment rule for parameter t_10:

$$t_10 = ModelValue_0$$
 (8)

8.8 Rule t_21

Rule t_21 is an assignment rule for parameter t_21 :

$$t_{21} = \begin{cases} 2 \cdot ModelValue_{0} & \text{if ModelValue}_{17} = 1\\ 0 & \text{otherwise} \end{cases}$$
 (9)

8.9 Rule t_32

Rule t_32 is an assignment rule for parameter t_32:

$$t_{-}32 = \begin{cases} 3 \cdot ModelValue_{-}0 & if ModelValue_{-}17 = 1\\ 0 & otherwise \end{cases}$$
 (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

No	Id	Name	Reaction Equation	SBO
1	G1GOA2	G1 -> G0 + A2	$G1 \xrightarrow{G1} G0 + A2$	
2	GOA2G1	G0 + A2 -> G1	$G0 + A2 \xrightarrow{G0, A2} G1$	
3	$G_{}G_{}rI$	G -> G + rI	$G0 \xrightarrow{G0} G0 + rI$	
4	G1G1rI	$G1 \rightarrow G1 + rI$	$G1 \xrightarrow{G1} G1 + rI$	
5	rA	rA ->	$rA \xrightarrow{rA} \emptyset$	
6	rA	-> rA	$\emptyset \longrightarrow rA$	
7	rI	rI ->	$rI \xrightarrow{rI} \emptyset$	
8	rArAA	$rA \rightarrow rA + A$	$rA \xrightarrow{rA} rA + A$	
9	I	I ->	$I \xrightarrow{I} \emptyset$	
10	rIrII	rI -> rI + I	$rI \xrightarrow{rI} rI + I$	
11	A	A ->	$A \xrightarrow{A} \emptyset$	
12	AIAI	$A + I \rightarrow AI$	$A + I \xrightarrow{A, I} AI$	
13	_2AA2	2 * A -> A2	$2 \stackrel{A}{\longrightarrow} A2$	
14	A2A	A2 -> 2 * A	$A2 \xrightarrow{A2} 2 A$	
15	AIAI	$AI \rightarrow A + I$	$AI \xrightarrow{AI} A + I$	
16	AI	AI ->	$AI \xrightarrow{AI} \emptyset$	
17	A2	A2 ->	$A2 \xrightarrow{A2} \emptyset$	

N⁰	Id	Name	Reaction Equation	SBO
18	G1A2G2	G1 + A2 -> G2	$G1 + A2 \xrightarrow{G1, A2} G2$	
19	G2G1A2	G2 -> G1 + A2	$G2 \xrightarrow{G2} G1 + A2$	
20	G2G2rI	$G2 \rightarrow G2 + rI$	$G2 \xrightarrow{G2} G2 + rI$	
21	G2A2G3	G2 + A2 -> G3	$G2 + A2 \xrightarrow{G2, A2} G3$	
22	G3A2	G3 -> G2 + A2	$G3 \xrightarrow{G3} G2 + A2$	
23	G3G3rI	$G3 \rightarrow G3 + rI$	$G3 \xrightarrow{G3} G3 + rI$	

9.1 Reaction G1____G0___A2

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

Name G1 -> G0 + A2

Reaction equation

$$G1 \xrightarrow{G1} G0 + A2 \tag{11}$$

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
GO	G0	
A2	A2	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \text{vol}(\text{yeast}) \cdot t_- 10 \cdot [\text{G1}] \tag{12}$$

9.2 Reaction GO___A2___G1

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

Name G0 + A2 -> G1

Reaction equation

$$G0 + A2 \xrightarrow{G0, A2} G1 \tag{13}$$

Reactants

Table 9: Properties of each reactant.

Id	Name	SBO
GO	G0	
A2	A2	

Modifiers

Table 10: Properties of each modifier.

Id	Name	SBO
GO	G0	
A2	A2	

Product

Table 11: Properties of each product.

Id	Name	SBO
G1	G1	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \text{vol}(\text{yeast}) \cdot \text{a_01} \cdot [\text{G0}] \cdot [\text{A2}]$$
 (14)

9.3 Reaction G____G__rI

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

Name $G \rightarrow G + rI$

Reaction equation

$$G0 \xrightarrow{G0} G0 + rI \tag{15}$$

Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
GO	G0	

Modifier

Table 13: Properties of each modifier.

Id	Name	SBO
GO	G0	

Products

Table 14: Properties of each product.

Id	Name	SBO
GO	G0	
rI	rI	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \text{vol}(\text{yeast}) \cdot \text{rho}_{-}f \cdot [G0]$$
 (16)

9.4 Reaction G1___G1__rI

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

Name $G1 \rightarrow G1 + rI$

Reaction equation

$$G1 \xrightarrow{G1} G1 + rI \tag{17}$$

Table 15: Properties of each reactant.

Id	Name	SBO
G1	G1	

Table 16: Properties of each modifier.

Id	Name	SBO
G1	G1	

Products

Table 17: Properties of each product.

Id	Name	SBO
G1	G1	
rI	rI	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \text{vol}(\text{yeast}) \cdot \text{rho}_{-}b \cdot [G1]$$
 (18)

9.5 Reaction rA___

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

Name $rA \rightarrow$

Reaction equation

$$rA \xrightarrow{rA} \emptyset$$
 (19)

Table 18: Properties of each reactant.

Id	Name	SBO
rA	rA	

Table 19: Properties of each modifier.

Id	Name	SBO
rA	rA	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \text{vol}(\text{yeast}) \cdot \text{delta}_{-m} \cdot [\text{rA}]$$
 (20)

9.6 Reaction ___rA

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

Name -> rA

Reaction equation

$$\emptyset \longrightarrow rA$$
 (21)

Product

Table 20: Properties of each product.

Id	Name	SBO
rA	rA	

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \text{vol}(\text{yeast}) \cdot \text{Constant_flux_irreversible}(\text{rho_0})$$
 (22)

Constant_flux_irreversible
$$(v) = v$$
 (23)

Constant_flux_irreversible
$$(v) = v$$
 (24)

9.7 Reaction rI___

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

Name $rI \rightarrow$

Reaction equation

$$rI \xrightarrow{rI} \emptyset$$
 (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

$$v_7 = \text{vol}(\text{yeast}) \cdot \text{delta}_{-m} \cdot [\text{rI}]$$
 (26)

9.8 Reaction rA___rA__A

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

Name $rA \rightarrow rA + A$

Reaction equation

$$rA \xrightarrow{rA} rA + A$$
 (27)

Table 23: Properties of each reactant.

Id	Name	SBO
rA	rA	

Table 24: Properties of each modifier.

Id	Name	SBO
rA	rA	

Products

Table 25: Properties of each product.

Id	Name	SBO
rA	rA	
Α	A	

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \text{vol}(\text{yeast}) \cdot \text{beta} \cdot [\text{rA}]$$
 (28)

9.9 Reaction I___

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

Name I ->

Reaction equation

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

Table 26: Properties of each reactant.

Id	Name	SBO
I	I	

Table 27: Properties of each modifier.

Id	Name	SBO
I	I	

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \text{vol}(\text{yeast}) \cdot \text{delta_p} \cdot [I]$$
 (30)

9.10 Reaction rI___rI__I

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

Name $rI \rightarrow rI + I$

Reaction equation

$$rI \xrightarrow{rI} rI + I$$
 (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

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

9.11 Reaction A___

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

Name $A \rightarrow$

Reaction equation

$$A \xrightarrow{A} \emptyset \tag{33}$$

Reactant

Table 31: Properties of each reactant.

Id	Name	SBO
Α	A	

Modifier

Table 32: Properties of each modifier.

Id	Name	SBO
Α	A	

Kinetic Law

Derived unit contains undeclared units

$$v_{11} = \text{vol}(\text{yeast}) \cdot \text{delta_p} \cdot [A]$$
 (34)

9.12 Reaction A...I....AI

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

Name A + I -> AI

Reaction equation

$$A + I \xrightarrow{A, I} AI \tag{35}$$

Reactants

Table 33: Properties of each reactant.

Id	Name	SBO
Α	A	
Ι	I	

Modifiers

Table 34: Properties of each modifier.

Id	Name	SBO
Α	A	
Ι	I	

Product

Table 35: Properties of each product.

Id	Name	SBO
AI	AI	

Kinetic Law

Derived unit contains undeclared units

$$v_{12} = \text{vol}(\text{yeast}) \cdot \text{gamma} \cdot [A] \cdot [I]$$
 (36)

9.13 Reaction _2___A___A2

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

Name 2 * A -> A2

Reaction equation

$$2A \xrightarrow{A} A2$$
 (37)

Reactant

Table 36: Properties of each reactant.

Id	Name	SBO
A	A	

Modifier

Table 37: Properties of each modifier.

Id	Name	SBO
A	A	

Product

Table 38: Properties of each product.

Id	Name	SBO
A2	A2	

Kinetic Law

Derived unit contains undeclared units

$$v_{13} = \text{vol}(\text{yeast}) \cdot \text{gamma} \cdot [A]^2$$
 (38)

9.14 Reaction A2___2_A

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

Name A2 -> 2 * A

Reaction equation

$$A2 \xrightarrow{A2} 2A \tag{39}$$

Reactant

Table 39: Properties of each reactant.

Id	Name	SBO
A2	A2	

Modifier

Table 40: Properties of each modifier.

Id	Name	SBO
A2	A2	

Product

Table 41: Properties of each product.

Id	Name	SBO
Α	A	

Kinetic Law

Derived unit contains undeclared units

$$v_{14} = \text{vol}(\text{yeast}) \cdot \text{epsilon}_{-1} \cdot [A2]$$
 (40)

9.15 Reaction AI___A__I

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

Name $AI \rightarrow A + I$

Reaction equation

$$AI \xrightarrow{AI} A + I$$
 (41)

Table 42: Properties of each reactant.

Id	Name	SBO
AI	AI	

Table 43: Properties of each modifier.

Id	Name	SBO
AI	AI	·

Products

Table 44: Properties of each product.

Id	Name	SBO
Α	A	
Ι	I	

Kinetic Law

Derived unit contains undeclared units

$$v_{15} = \text{vol}(\text{yeast}) \cdot \text{epsilon} \cdot [\text{AI}]$$
 (42)

9.16 Reaction AI___

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

Name AI ->

Reaction equation

$$AI \xrightarrow{AI} \emptyset$$
 (43)

Table 45: Properties of each reactant.

Id	Name	SBO
AI	AI	

Table 46: Properties of each modifier.

Id	Name	SBO
AI	AI	

Kinetic Law

Derived unit contains undeclared units

$$v_{16} = \text{vol}(\text{yeast}) \cdot \text{delta_p} \cdot [\text{AI}]$$
 (44)

9.17 Reaction A2___

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

Name $A2 \rightarrow$

Reaction equation

$$A2 \xrightarrow{A2} \emptyset \tag{45}$$

Reactant

Table 47: Properties of each reactant.

Id	Name	SBO
A2	A2	

Modifier

Table 48: Properties of each modifier.

Id	Name	SBO
A2	A2	

Kinetic Law

Derived unit contains undeclared units

$$v_{17} = \text{vol}(\text{yeast}) \cdot \text{delta_p} \cdot [\text{A2}] \tag{46}$$

9.18 Reaction G1___A2___G2

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

Name G1 + A2 -> G2

Reaction equation

$$G1 + A2 \xrightarrow{G1, A2} G2 \tag{47}$$

Reactants

Table 49: Properties of each reactant.

Id	Name	SBO
G1	G1	
A2	A2	

Modifiers

Table 50: Properties of each modifier.

Id	Name	SBO
G1	G1	
A2	A2	

Product

Table 51: Properties of each product.

Id	Name	SBO
G2	G2	

Kinetic Law

Derived unit contains undeclared units

$$v_{18} = \text{vol}(\text{yeast}) \cdot \text{a}_{-}12 \cdot [\text{G1}] \cdot [\text{A2}] \tag{48}$$

9.19 Reaction G2___G1__A2

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

Name G2 -> G1 + A2

Reaction equation

$$G2 \xrightarrow{G2} G1 + A2 \tag{49}$$

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	
A2	A2	

Kinetic Law

Derived unit contains undeclared units

$$v_{19} = \text{vol}(\text{yeast}) \cdot \text{t}_{-}21 \cdot [\text{G2}] \tag{50}$$

9.20 Reaction G2____G2___rI

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

Name $G2 \rightarrow G2 + rI$

Reaction equation

$$G2 \xrightarrow{G2} G2 + rI \tag{51}$$

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	
rI	rI	

Kinetic Law

Derived unit contains undeclared units

$$v_{20} = \text{vol}(\text{yeast}) \cdot \text{rho}_{-}\text{b} \cdot [\text{G2}]$$
 (52)

9.21 Reaction G2___A2___G3

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

Name G2 + A2 -> G3

Reaction equation

$$G2 + A2 \xrightarrow{G2, A2} G3 \tag{53}$$

Reactants

Table 58: Properties of each reactant.

Id	Name	SBO
G2	G2	
A2	A2	

Modifiers

Table 59: Properties of each modifier.

Id	Name	SBO
G2	G2	
A2	A2	

Product

Table 60: Properties of each product.

	_	
Id	Name	SBO
G3	G3	

Kinetic Law

Derived unit contains undeclared units

$$v_{21} = \text{vol}(\text{yeast}) \cdot \text{a}_{23} \cdot [\text{G2}] \cdot [\text{A2}]$$
(54)

9.22 Reaction G3____G2___A2

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

Name G3 -> G2 + A2

Reaction equation

$$G3 \xrightarrow{G3} G2 + A2 \tag{55}$$

Table 61: Properties of each reactant.

Id	Name	SBO
G3	G3	

Table 62: Properties of each modifier.

Id	Name	SBO
G3	G3	

Products

Table 63: Properties of each product.

Id	Name	SBO
G2	G2	
A2	A2	

Kinetic Law

Derived unit contains undeclared units

$$v_{22} = \text{vol}(\text{yeast}) \cdot \text{t}_{-}32 \cdot [\text{G3}]$$
 (56)

9.23 Reaction G3____G3___rI

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

Name $G3 \rightarrow G3 + rI$

Reaction equation

$$G3 \xrightarrow{G3} G3 + rI \tag{57}$$

Table 64: Properties of each reactant.

Id	Name	SBO
G3	G3	

Table 65: Properties of each modifier.

Id	Name	SBO
G3	G3	

Products

Table 66: Properties of each product.

Id	Name	SBO
G3	G3	
rI	rI	

Kinetic Law

Derived unit contains undeclared units

$$v_{23} = \text{vol}(\text{yeast}) \cdot \text{rho}_{-}\text{b} \cdot [\text{G3}]$$
 (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 GO

Name G0

SBO:0000196 concentration of an entity pool

Initial concentration 1 item · dimensionless⁻¹

This species takes part in six reactions (as a reactant in G0__A2__G1, G___G__rI and as a product in G1__G0__A2, G___rI and as a modifier in G0__A2__G1, G___G__rI).

$$\frac{d}{dt}G0 = |v_1| + |v_3| - |v_2| - |v_3| \tag{59}$$

10.2 Species G1

Name G1

SBO:0000196 concentration of an entity pool

Initial concentration 0 item · dimensionless⁻¹

This species takes part in nine reactions (as a reactant in G1___G0__A2, G1___G1__rI, G1__-A2___G2 and as a product in G0__A2___G1, G1___rI, G2___G1__A2 and as a modifier in G1___G0__A2, G1___G1__rI, G1__A2___G2).

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

10.3 Species rA

Name rA

SBO:0000278 messenger RNA

Initial concentration 0 item · dimensionless⁻¹

This species takes part in six reactions (as a reactant in rA___, rA___rA___A and as a product in ____rA, rA___rA___A and as a modifier in rA___, rA___rA___A).

$$\frac{d}{dt}rA = v_6 + v_8 - v_5 - v_8 \tag{61}$$

10.4 Species I

Name I

SBO:0000020 inhibitor

Initial concentration 0 item · dimensionless⁻¹

This species takes part in six reactions (as a reactant in I_{--} , $A_{--}I_{--}$ AI and as a product in rI_{--} I, rI_{--} I, and as a modifier in I_{--} , A_{--} I...AI).

$$\frac{\mathrm{d}}{\mathrm{d}t}I = |v_{10}| + |v_{15}| - |v_{9}| - |v_{12}| \tag{62}$$

10.5 Species rI

Name rI

SBO:0000278 messenger RNA

Initial concentration 0 item · dimensionless⁻¹

This species takes part in nine reactions (as a reactant in rI___, rI___rI__I and as a product in G___G__rI, G1___rI, rI___rI__I, G2___G2__rI, G3___rI and as a modifier in rI__, rI___rI__I).

$$\frac{\mathrm{d}}{\mathrm{d}t}rI = v_3 + v_4 + v_{10} + v_{20} + v_{23} - v_7 - v_{10}$$
(63)

10.6 Species A

Name A

SBO:0000459 stimulator

Initial concentration 0 item ⋅ dimensionless⁻¹

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

10.7 Species AI

Name AI

SBO:0000609 heterodimer

Initial concentration 0 item · dimensionless⁻¹

This species takes part in five reactions (as a reactant in $AI_{---}A_{---}I$, AI_{---} and as a product in $A_{---}I_{---}AI$ and as a modifier in $AI_{---}A_{---}I$, $AI_{---}I_{---}I$.

$$\frac{d}{dt}AI = |v_{12}| - |v_{15}| - |v_{16}| \tag{65}$$

10.8 Species A2

Name A2

SBO:0000608 homodimer

Initial concentration 0 item ⋅ dimensionless⁻¹

This species takes part in 14 reactions (as a reactant in G0__A2___G1, A2___2__A, A2___, G1__A2___G2, G2__A2___G3 and as a product in G1___G0__A2, _2__A__A2, G2___G1__A2, G3___G2__A2 and as a modifier in G0__A2___G1, A2___2_A, A2___, G1__A2___G2, G2__A2___G3).

$$\frac{\mathrm{d}}{\mathrm{d}t}A2 = |v_1| + |v_{13}| + |v_{19}| + |v_{22}| - |v_2| - |v_{14}| - |v_{17}| - |v_{18}| - |v_{21}|$$
(66)

10.9 Species G2

Name G2

SBO:0000196 concentration of an entity pool

Initial concentration 0 item · dimensionless⁻¹

This species takes part in nine reactions (as a reactant in G2___G1__A2, G2___G2__rI, G2__-A2___G3 and as a product in G1__A2___G2, G2___rI, G3___G2__A2 and as a modifier in G2___G1__A2, G2___G2__rI, G2__A2___G3).

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

10.10 Species G3

Name G3

SBO:0000196 concentration of an entity pool

Initial concentration 0 item · dimensionless⁻¹

This species takes part in six reactions (as a reactant in G3___G2__A2, G3___g3__rI and as a product in G2__A2__G3, G3___rI and as a modifier in G3___G2__A2, G3___G3__rI).

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

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: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:0000459 stimulator:** Substance that accelerates the velocity of a chemical reaction without itself being consumed or transformed.
- **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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