SBML Model Report

Model name: "Vilar2002_Oscillator"

May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 3 format. This model was created by the following two authors: Nicolas Le Novre[1] and Bruce Shapiro[2] at June 30th 2005 at 10:20 a. m. and last time modified at June third 2013 at 1:58 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	10
events	0	constraints	0
reactions	16	function definitions	0
global parameters	0	unit definitions	1
rules	0	initial assignments	0

Model Notes

Minimal Model for Circadian Oscillations
Minimal Model for Circadian Oscillations

Citation

[1]EMBL-EBI, lenov@ebi.ac.uk
[2]Jet Propulsion Laboratory, bshapiro@caltech.edu

Vilar JMG, Kueh HY, Barkai N, Leibler S, (2002). Mechanisms of noise resistance in genetic oscillators, PNAS, 99(9):5988-5992. http://www.pnas.org/cgi/content/abstract/99/9/5988

Description
A minimal model of genomically based oscillation, based on two mutually interacting genes, an activator and a repressor. Postive feedback is provided by the activator protein, which binds to the promotors of both the activator and the repressor genes. Negative feedback is provided by the repressor protein which binds to the activator protein.

Rateconstant	Reaction
alphaA=50	DA->DA+MA
alphaAp=500	DAp->DAp+MA
alphaR=0.01	DR->DR+MR
alphaRp=50	DRp->DRp+MR
betaA=50	MA->A+MA
betaR=5	MR->MR+R
gammaA=1	A+DA->DAp
gammaC=2	A+R->C
gammaR=1	A+DR->DRp
deltaA=1	A->EmptySet
deltaA=1	C->R
deltaMA=10	MA->EmptySet
deltaMR=0.5	MR->EmptySet
deltaR=0.2	R->EmptySet
thetaA=50	DAp->A+DA
thetaR=100	DRp->A+DR

Variable	IC	ODE
A	0	A'[t]==-(deltaA*A[t])-gammaA*A[t]*DA[t]+thetaA*DAp[t]-gammaR*A[t]*DR[t]+thetaR*DRp[t]+betaA*MA gammaC*A[t]*R[t]
C	0	C'[t]==-(deltaA*C[t])+gammaC*A[t]*R[t]
DA	1	DA'[t]==-(gammaA*A[t]*DA[t])+thetaA*DAp[t]

DAp	0	DAp'[t]==gammaA*A[t]*DA[t]-thetaA*DAp[t]
DR	1	DR'[t]==-(gammaR*A[t]*DR[t])+thetaR*DRp[t]
DRp	0	DRp'[t]==gammaR*A[t]*DR[t]-thetaR*DRp[t]
MA	0	MA'[t]==alphaA*DA[t]+alphaAp*DAp[t]-deltaMA*MA[t]
MR	0	MR'[t]==alphaR*DR[t]+alphaRp*DRp[t]-deltaMR*MR[t]
R	0	R'[t]==deltaA*C[t]+betaR*MR[t]-deltaR*R[t]-gammaC*A[t]*R[t]

Generated by Cellerator Version 1.0 update 2.1127 using Mathematica 4.2 for Mac OS X (June 4, 2002), November 27, 2002 12:17:46, using (PowerMac,PowerPC,Mac OS X,MacOSX,Darwin)

author=B.E.Shapiro

2 Unit Definitions

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

2.1 Unit `time`

Name hour

Definition 3600 s

2.2 Unit `substance`

Notes Mole is the predefined SBML unit for `substance`.

Definition mol

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 6: Properties of all compartments.

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

3.1 Compartment deterministicOscillator

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

4 Species

This model contains ten species. The boundary condition of one of these species is set to `true` so that this species' amount cannot be changed by any reaction. Section 6 provides further details and the derived rates of change of each species.

Table 7: Properties of each species.

Id	Name	Compartment	Derived Unit	Constant	Boundary Condition
EmptySet		deterministicOscillator	mol	☐	☑
A		deterministicOscillator	mol	☐	☐
C		deterministicOscillator	mol	☐	☐
DA		deterministicOscillator	mol	☐	☐
DAp		deterministicOscillator	mol	☐	☐
DR		deterministicOscillator	mol	☐	☐
DRp		deterministicOscillator	mol	☐	☐
MA		deterministicOscillator	mol	☐	☐
MR		deterministicOscillator	mol	☐	☐
R		deterministicOscillator	mol	☐	☐

5 Reactions

This model contains 16 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 8: Overview of all reactions

№	Id	Name	Reaction Equation	SBO
1	Reaction1		$A + R \longrightarrow C$	
2	Reaction2		$A \longrightarrow EmptySet$	
3	Reaction3		$C \longrightarrow R$	
4	Reaction4		$R \longrightarrow EmptySet$	
5	Reaction5		$A + DA \longrightarrow DAp$	
6	Reaction6		$DAp \longrightarrow A + DA$	
7	Reaction7		$DA \longrightarrow DA + MA$	
8	Reaction8		$DAp \longrightarrow DAp + MA$	
9	Reaction9		$MA \longrightarrow EmptySet$	
10	Reaction10		$MA \longrightarrow A + MA$	
11	Reaction11		$A + DR \longrightarrow DRp$	
12	Reaction12		$DRp \longrightarrow A + DR$	
13	Reaction13		$DR \longrightarrow DR + MR$	
14	Reaction14		$DRp \longrightarrow DRp + MR$	
15	Reaction15		$MR \longrightarrow EmptySet$	
16	Reaction16		$MR \longrightarrow MR + R$	

5.1 Reaction Reaction1

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

Reaction equation

$$\mathrm{A} + \mathrm{R} \longrightarrow \mathrm{C} \tag{1}$$

Reactants

Table 9: Properties of each reactant.

Id	Name	SBO
A		
R		

Product

Table 10: Properties of each product.

Id	Name	SBO
C		

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \mathrm{A} \cdot \mathrm{R} \cdot \mathrm{gammaC} \tag{2}$$

Table 11: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
gammaC			**2.0**		☑

5.2 Reaction Reaction2

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

Reaction equation

$$\mathrm{A} \longrightarrow \mathrm{EmptySet} \tag{3}$$

Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
A		

Product

Table 13: Properties of each product.

Id	Name	SBO
EmptySet		

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \mathrm{A} \cdot \mathrm{deltaA} \tag{4}$$

Table 14: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
deltaA			**1.0**		☑

5.3 Reaction Reaction3

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

Reaction equation

$$\mathrm{C} \longrightarrow \mathrm{R} \tag{5}$$

Reactant

Table 15: Properties of each reactant.

Id	Name	SBO
C		

Product

Table 16: Properties of each product.

Id	Name	SBO
R		

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \mathrm{C} \cdot \mathrm{deltaA} \tag{6}$$

Table 17: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
deltaA			**1.0**		☑

5.4 Reaction Reaction4

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

Reaction equation

$$\mathrm{R} \longrightarrow \mathrm{EmptySet} \tag{7}$$

Reactant

Table 18: Properties of each reactant.

Id	Name	SBO
R		

Product

Table 19: Properties of each product.

Id	Name	SBO
EmptySet		

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \mathrm{R} \cdot \mathrm{deltaR} \tag{8}$$

Table 20: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
deltaR			**0.2**		☑

5.5 Reaction Reaction5

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

Reaction equation

$$\mathrm{A} + \mathrm{DA} \longrightarrow \mathrm{DAp} \tag{9}$$

Reactants

Table 21: Properties of each reactant.

Id	Name	SBO
A		
DA		

Product

Table 22: Properties of each product.

Id	Name	SBO
DAp		

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \mathrm{A} \cdot \mathrm{DA} \cdot \mathrm{gammaA} \tag{10}$$

Table 23: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
gammaA			**1.0**		☑

5.6 Reaction Reaction6

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

Reaction equation

$$\mathrm{DAp} \longrightarrow \mathrm{A} + \mathrm{DA} \tag{11}$$

Reactant

Table 24: Properties of each reactant.

Id	Name	SBO
DAp		

Products

Table 25: Properties of each product.

Id	Name	SBO
A		
DA		

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \mathrm{DAp} \cdot \mathrm{thetaA} \tag{12}$$

Table 26: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
thetaA			50.0		☑

5.7 Reaction Reaction7

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

Reaction equation

$$\mathrm{DA} \longrightarrow \mathrm{DA} + \mathrm{MA} \tag{13}$$

Reactant

Table 27: Properties of each reactant.

Id	Name	SBO
DA		

Products

Table 28: Properties of each product.

Id	Name	SBO
DA		
MA		

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \mathrm{DA} \cdot \mathrm{alphaA} \tag{14}$$

Table 29: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
alphaA			50.0		☑

5.8 Reaction Reaction8

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

Reaction equation

$$\mathrm{DAp} \longrightarrow \mathrm{DAp} + \mathrm{MA} \tag{15}$$

Reactant

Table 30: Properties of each reactant.

Id	Name	SBO
DAp		

Products

Table 31: Properties of each product.

Id	Name	SBO
DAp		
MA		

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \mathrm{DAp} \cdot \mathrm{alphaAp} \tag{16}$$

Table 32: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
alphaAp			**500.0**		☑

5.9 Reaction Reaction9

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

Reaction equation

$$\mathrm{MA} \longrightarrow \mathrm{EmptySet} \tag{17}$$

Reactant

Table 33: Properties of each reactant.

Id	Name	SBO
MA		

Product

Table 34: Properties of each product.

Id	Name	SBO
EmptySet		

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \mathrm{MA} \cdot \mathrm{deltaMA} \tag{18}$$

Table 35: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
deltaMA			**10.0**		☑

5.10 Reaction Reaction10

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

Reaction equation

$$\mathrm{MA} \longrightarrow \mathrm{A} + \mathrm{MA} \tag{19}$$

Reactant

Table 36: Properties of each reactant.

Id	Name	SBO
MA		

Products

Table 37: Properties of each product.

Id	Name	SBO
A		
MA		

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = \mathrm{MA} \cdot \mathrm{betaA} \tag{20}$$

Table 38: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
betaA			**50.0**		☑

5.11 Reaction Reaction11

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

Reaction equation

$$\mathrm{A} + \mathrm{DR} \longrightarrow \mathrm{DRp} \tag{21}$$

Reactants

Table 39: Properties of each reactant.

Id	Name	SBO
A		
DR		

Product

Table 40: Properties of each product.

Id	Name	SBO
DRp		

Kinetic Law

Derived unit contains undeclared units

$$v_{11} = \mathrm{A} \cdot \mathrm{DR} \cdot \mathrm{gammaR} \tag{22}$$

Table 41: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
gammaR			**1.0**		☑

5.12 Reaction Reaction12

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

Reaction equation

$$\mathrm{DRp} \longrightarrow \mathrm{A} + \mathrm{DR} \tag{23}$$

Reactant

Table 42: Properties of each reactant.

Id	Name	SBO
DRp		

Products

Table 43: Properties of each product.

Id	Name	SBO
A		
DR		

Id	Name	SBO

Kinetic Law

Derived unit contains undeclared units

$$v_{12} = \mathrm{DRp} \cdot \mathrm{thetaR} \tag{24}$$

Table 44: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
thetaR			**100.0**		☑

5.13 Reaction Reaction13

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

Reaction equation

$$\mathrm{DR} \longrightarrow \mathrm{DR} + \mathrm{MR} \tag{25}$$

Reactant

Table 45: Properties of each reactant.

Id	Name	SBO
DR		

Products

Table 46: Properties of each product.

Id	Name	SBO
DR		
MR		

Kinetic Law

Derived unit contains undeclared units

$$v_{13} = \mathrm{DR} \cdot \mathrm{alphaR} \quad \textbf{(26)}$$

Table 47: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
alphaR			**0.01**		☑

5.14 Reaction Reaction14

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

Reaction equation

$$\mathrm{DRp} \longrightarrow \mathrm{DRp} + \mathrm{MR} \quad (27)$$

Reactant

Table 48: Properties of each reactant.

Id	Name	SBO
DRp		

Products

Table 49: Properties of each product.

Id	Name	SBO
DRp		
MR		

Kinetic Law

Derived unit contains undeclared units

$$v_{14} = \mathrm{DRp} \cdot \mathrm{alphaRp} \quad \textbf{(28)}$$

Table 50: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
alphaRp			**50.0**		☑

5.15 Reaction Reaction15

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

Reaction equation

$$\mathrm{MR} \longrightarrow \mathrm{EmptySet} \tag{29}$$

Reactant

Table 51: Properties of each reactant.

Id	Name	SBO
MR		

Product

Table 52: Properties of each product.

Id	Name	SBO
EmptySet		

Kinetic Law

Derived unit contains undeclared units

$$v_{15} = \mathrm{MR} \cdot \mathrm{deltaMR} \tag{30}$$

Table 53: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
deltaMR			**0.5**		☑

5.16 Reaction Reaction16

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

Reaction equation

$$\mathrm{MR} \longrightarrow \mathrm{MR} + \mathrm{R} \tag{31}$$

Reactant

Table 54: Properties of each reactant.

Id	Name	SBO
MR		

Products

Table 55: Properties of each product.

Id	Name	SBO
MR		
R		

Kinetic Law

Derived unit contains undeclared units

$$v_{16} = \mathrm{MR} \cdot \mathrm{betaR} \tag{32}$$

Table 56: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
betaR			5.0		☑

6 Derived Rate Equations

When interpreted as an ordinary differential equation framework, this model implies the following set of equations for the rates of change of each species.

Identifiers for kinetic laws highlighted in gray cannot be verified to evaluate to units of SBML `substance` per `time`. As a result, some SBML interpreters may not be able to verify the consistency of the units on quantities in the model. Please check if

- **parameters without an unit definition are involved or**
- **volume correction is necessary because the `hasOnlySubstanceUnits` flag may be set to `false` and `spacialDimensions`> 0 for certain species.**

6.1 Species EmptySet

Initial amount 0 mol

This species takes part in four reactions (as a product in Reaction2, Reaction4, Reaction9, Reaction15), which do not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{EmptySet} = 0 \tag{33}$$

6.2 Species A

Initial amount 0 mol

This species takes part in seven reactions (as a reactant in Reaction1, Reaction2, Reaction5, Reaction11 and as a product in Reaction6, Reaction10, Reaction12).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{A} = v_6 + v_{10} + v_{12} - v_1 - v_2 - v_5 - v_{11} \tag{34}$$

6.3 Species C

Initial amount 0 mol

This species takes part in two reactions (as a reactant in Reaction3 and as a product in Reaction1).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C} = v_1 - v_3 \tag{35}$$

6.4 Species DA

Initial amount 1 mol

This species takes part in four reactions (as a reactant in Reaction5, Reaction7 and as a product in Reaction6, Reaction7).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{DA} = v_6 + v_7 - v_5 - v_7 \tag{36}$$

6.5 Species DAp

Initial amount 0 mol

This species takes part in four reactions (as a reactant in Reaction6, Reaction8 and as a product in Reaction5, Reaction8).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{DAp} = v_5 + v_8 - v_6 - v_8 \tag{37}$$

6.6 Species DR

Initial amount 1 mol

This species takes part in four reactions (as a reactant in Reaction11, Reaction13 and as a product in Reaction12, Reaction13).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{DR} = v_{12} + v_{13} - v_{11} - v_{13} \tag{38}$$

6.7 Species DRp

Initial amount 0 mol

This species takes part in four reactions (as a reactant in Reaction12, Reaction14 and as a product in Reaction11, Reaction14).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{DRp} = v_{11} + v_{14} - v_{12} - v_{14} \tag{39}$$

6.8 Species MA

Initial amount 0 mol

This species takes part in five reactions (as a reactant in Reaction9, Reaction10 and as a product in Reaction7, Reaction8, Reaction10).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{MA} = v_{7} + v_{8} + v_{10} - v_{9} - v_{10} \tag{40}$$

6.9 Species MR

Initial amount 0 mol

This species takes part in five reactions (as a reactant in Reaction15, Reaction16 and as a product in Reaction13, Reaction14, Reaction16).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{MR} = v_{13} + v_{14} + v_{16} - v_{15} - v_{16} \tag{41}$$

6.10 Species R

Initial amount 0 mol

This species takes part in four reactions (as a reactant in Reaction1, Reaction4 and as a product in Reaction3, Reaction16).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{R} = v_{3} + v_{16} - v_{1} - v_{4} \tag{42}$$

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