SBML Model Report

Model name: "Goldbeter1995_CircClock"

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1 General Overview

This is a document in SBML Level 2 Version 1 format. This model was created by the following two authors: Nicolas Le Novre[1] and Bruce Shapiro[2] at June 29th 2005 at 10:17 a. m. and last time modified at February 25th 2015 at 1:08 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	3
species types	0	species	7
events	0	constraints	0
reactions	10	function definitions	0
global parameters	0	unit definitions	2
rules	1	initial assignments	0

Model Notes

[1]EMBL-EBI, lenov@ebi.ac.uk
[2]NASA Jet Propulsion Laboratory, bshapiro@jpl.nasa.gov

commercially or not, in a restricted way or not.

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2 Unit Definitions

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

2.1 Unit `substance`

Name micromole (default)

Notes Default unit of substance redefined to micromole by comparison with the article. Nicolas Le Novere

Definition µmol

2.2 Unit `time`

Name heure (default)

Notes Default unit of time redefined to hour by comparison with the article. Nicolas Le Novere

Definition 3600 s

2.3 Unit `volume`

Notes Litre is the predefined SBML unit for `volume`.

Definition l

2.4 Unit `area`

Notes Square metre is the predefined SBML unit for `area` since SBML Level 2 Version 1.

Definition m^2

2.5 Unit `length`

Notes Metre is the predefined SBML unit for `length` since SBML Level 2 Version 1.

Definition m

3 Compartments

This model contains three compartments.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
default			3	10^{-15}	l	☑	
CYTOPLASM			3	10^{-15}	l	☑	default
compartment_0000004	NUCLEUS		3	10^{-15}	l	☑	CYTOPLASM

3.1 Compartment default

This is a three dimensional compartment with a constant size of 10^{-15} litre.

3.2 Compartment CYTOPLASM

This is a three dimensional compartment with a constant size of 10^{-15} litre, which is surrounded by default.

3.3 Compartment compartment_0000004

This is a three dimensional compartment with a constant size of 10^{-15} litre, which is surrounded by CYTOPLASM.

Name NUCLEUS

4 Species

This model contains seven 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 7 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
`EmptySet`		`default`	$\mu mol \cdot l^{-1}$	☑	☑
`M`	PER mRNA	`CYTOPLASM`	$\mu mol \cdot l^{-1}$	☐	☐
`P0`	unphosphorylated PER	`CYTOPLASM`	$\mu mol \cdot l^{-1}$	☐	☐
`P1`	monophosphorylated PER	`CYTOPLASM`	$\mu mol \cdot l^{-1}$	☐	☐
`P2`	biphosphorylated PER	`CYTOPLASM`	$\mu mol \cdot l^{-1}$	☐	☐
`Pn`	nuclear PER	`compartment_0000004`	$\mu mol \cdot l^{-1}$	☐	☐
`Pt`	total PER	`CYTOPLASM`	$\mu mol \cdot l^{-1}$	☐	☐

5 Rule

This is an overview of one rule.

5.1 Rule `Pt`

Rule `Pt` is an assignment rule for species `Pt`:

$$\mathrm{Pt} = [\mathrm{P0}] + [\mathrm{P1}] + [\mathrm{P2}] + [\mathrm{Pn}] \tag{1}$$

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

Notes Conversion to number of molecules removed to give result in micromoles.

Pn added to formula for consistency with reference. Bruce Shapiro

6 Reactions

This model contains ten 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 4: Overview of all reactions

№	Id	Name	Reaction Equation	SBO
1	rM	transcription of PER	EmptySet $\xrightarrow{\text{Pn}}$ M	
2	rTL	translation of PER	EmptySet $\xrightarrow{\text{M}}$ P0	
3	rP01	first phosphorylation of PER	P0 $\longrightarrow$ P1	
4	rP10	removal of the first PER phosphate	P1 $\longrightarrow$ P0	
5	rP12	second phosphorylation of PER	P1 $\longrightarrow$ P2	
6	rP21	removal of the second PER phosphate	P2 $\longrightarrow$ P1	
7	rP2n	translocation of PER to the nucleus	P2 $\longrightarrow$ Pn	
8	rPn2	translocation of PER to the cytoplasm	Pn $\longrightarrow$ P2	
9	rmRNAd	degradation of PER mRNA	M $\longrightarrow$ EmptySet	
10	rVd	degradation of PER	P2 $\longrightarrow$ EmptySet	

6.1 Reaction rM

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

Name transcription of PER

Reaction equation

$$\text{EmptySet} \xrightarrow{\text{Pn}} \text{M} \tag{2}$$

Reactant

Table 5: Properties of each reactant.

Id	Name	SBO
EmptySet		

Modifier

Table 6: Properties of each modifier.

Id	Name	SBO
Pn	nuclear PER	

Product

Table 7: Properties of each product.

Id	Name	SBO
M	PER mRNA	

Kinetic Law

Notes Formula modified to give units of substance/time Bruce Shapiro

Derived unit contains undeclared units

$$v_1 = \frac{\text{vol}\,(\text{default}) \cdot \text{Vs} \cdot \text{KI}^{\text{n}}}{\text{KI}^{\text{n}} + [\text{Pn}]^{\text{n}}} \tag{3}$$

Table 8: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vs			0.76		☑
KI			1.00		☑
n			4.00		☑

6.2 Reaction rTL

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

Name translation of PER

Reaction equation

$$\text{EmptySet} \xrightarrow{\text{M}} \text{P0} \tag{4}$$

Reactant

Table 9: Properties of each reactant.

Id	Name	SBO
EmptySet		

Modifier

Table 10: Properties of each modifier.

Id	Name	SBO
M	PER mRNA	

Product

Table 11: Properties of each product.

Id	Name	SBO
P0	unphosphorylated PER	

Kinetic Law

Notes Formula modified to give units of substance/time Bruce Shapiro

Derived unit contains undeclared units

$$v_2 = \mathrm{ks} \cdot [\mathrm{M}] \cdot \mathrm{vol}\,(\mathrm{default}) \tag{5}$$

Table 12: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
ks			0.38		☑

6.3 Reaction rP01

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

Name first phosphorylation of PER

Reaction equation

$$\mathrm{P0} \longrightarrow \mathrm{P1} \tag{6}$$

Reactant

Table 13: Properties of each reactant.

Id	Name	SBO
P0	unphosphorylated PER	

Product

Table 14: Properties of each product.

Id	Name	SBO
P1	monophosphorylated PER	

Kinetic Law

Notes Formula modified to give units of substance/time Bruce Shapiro

Derived unit contains undeclared units

$$v_3 = \frac{\mathrm{vol}\,(\mathrm{CYTOPLASM}) \cdot \mathrm{V1} \cdot [\mathrm{P0}]}{\mathrm{K1} + [\mathrm{P0}]} \tag{7}$$

Table 15: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V1			3.2		☑
K1			2.0		☑

6.4 Reaction rP10

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

Name removal of the first PER phosphate

Reaction equation

$$\mathrm{P1} \longrightarrow \mathrm{P0} \tag{8}$$

Reactant

Table 16: Properties of each reactant.

Id	Name	SBO
P1	monophosphorylated PER	

Product

Table 17: Properties of each product.

Id	Name	SBO
P0	unphosphorylated PER	

Kinetic Law

Notes Formula modified to give units of substance/time Bruce Shapiro

Derived unit contains undeclared units

$$v_4 = \frac{\mathrm{vol}\left(\mathrm{CYTOPLASM}\right) \cdot \mathrm{V2} \cdot [\mathrm{P1}]}{\mathrm{K2} + [\mathrm{P1}]} \tag{9}$$

Table 18: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V2			1.58		☑
K2			2.00		☑

6.5 Reaction rP12

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

Name second phosphorylation of PER

Reaction equation

$$\mathrm{P1} \longrightarrow \mathrm{P2} \tag{10}$$

Reactant

Table 19: Properties of each reactant.

Id	Name	SBO
P1	monophosphorylated PER	

Product

Table 20: Properties of each product.

Id	Name	SBO
P2	biphosphorylated PER	

Kinetic Law

Notes Formula modified to give units of substance/time Bruce Shapiro

Derived unit contains undeclared units

$$v_5 = \frac{\mathrm{vol}\left(\mathrm{CYTOPLASM}\right) \cdot \mathrm{V3} \cdot [\mathrm{P1}]}{\mathrm{K3} + [\mathrm{P1}]} \tag{11}$$

Table 21: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V3			5.0		☑
K3			2.0		☑

6.6 Reaction rP21

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

Name removal of the second PER phosphate

Reaction equation

$$\mathrm{P2} \longrightarrow \mathrm{P1} \tag{12}$$

Reactant

Table 22: Properties of each reactant.

Id	Name	SBO
P2	biphosphorylated PER	

Product

Table 23: Properties of each product.

Id	Name	SBO
P1	monophosphorylated PER	

Kinetic Law

Notes Formula modified to give units of substance/time Bruce Shapiro

Derived unit contains undeclared units

$$v_6 = \frac{\mathrm{vol}\left(\mathrm{CYTOPLASM}\right) \cdot \mathrm{V4} \cdot [\mathrm{P2}]}{\mathrm{K4} + [\mathrm{P2}]} \tag{13}$$

Table 24: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V4			2.5		☑
K4			2.0		☑

6.7 Reaction rP2n

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

Name translocation of PER to the nucleus

Reaction equation

$$\mathrm{P2} \longrightarrow \mathrm{Pn} \tag{14}$$

Reactant

Table 25: Properties of each reactant.

Id	Name	SBO
P2	biphosphorylated PER	

Product

Table 26: Properties of each product.

Id	Name	SBO
Pn	nuclear PER	

Kinetic Law

Notes Formula modified to give units of substance/time Bruce Shapiro

Derived unit contains undeclared units

$$v_7 = \mathrm{k1} \cdot [\mathrm{P2}] \cdot \mathrm{vol}\,(\mathrm{CYTOPLASM}) \tag{15}$$

Table 27: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1			1.9		☑

6.8 Reaction rPn2

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

Name translocation of PER to the cytoplasm

Reaction equation

$$\mathrm{Pn} \longrightarrow \mathrm{P2} \tag{16}$$

Reactant

Table 28: Properties of each reactant.

Id	Name	SBO
Pn	nuclear PER	

Product

Table 29: Properties of each product.

Id	Name	SBO
P2	biphosphorylated PER	

Kinetic Law

Notes Formula modified to give units of substance/time Bruce Shapiro

Derived unit contains undeclared units

$$v_8 = \mathrm{k2} \cdot [\mathrm{Pn}] \cdot \mathrm{vol}\,(\mathrm{compartment\_0000004}) \tag{17}$$

Table 30: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k2			1.3		☑

6.9 Reaction rmRNAd

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

Name degradation of PER mRNA

Reaction equation

$$\mathrm{M} \longrightarrow \mathrm{EmptySet} \tag{18}$$

Reactant

Table 31: Properties of each reactant.

Id	Name	SBO
M	PER mRNA	

Product

Table 32: Properties of each product.

Id	Name	SBO
EmptySet		

Kinetic Law

Notes Formula modified to give units of substance/time Bruce Shapiro

Derived unit contains undeclared units

$$v_9 = \frac{\mathrm{Vm} \cdot [\mathrm{M}] \cdot \mathrm{vol}\,(\mathrm{CYTOPLASM})}{\mathrm{Km} + [\mathrm{M}]} \tag{19}$$

Table 33: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Km			0.50		☑
Vm			0.65		☑

6.10 Reaction rVd

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

Name degradation of PER

Reaction equation

$$\mathrm{P2} \longrightarrow \mathrm{EmptySet} \tag{20}$$

Reactant

Table 34: Properties of each reactant.

Id	Name	SBO
P2	biphosphorylated PER	

Product

Table 35: Properties of each product.

Id	Name	SBO
EmptySet		

Kinetic Law

Notes Formula modified to give units of substance/time Bruce Shapiro

Derived unit contains undeclared units

$$v_{10} = \frac{\text{vol}\,(\text{CYTOPLASM}) \cdot \text{Vd} \cdot [\text{P2}]}{\text{Kd} + [\text{P2}]} \tag{21}$$

Table 36: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Vd			0.95		☑
Kd			0.20		☑

7 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.

7.1 Species EmptySet

Notes boundaryCondition changed from default (i.e. false) to true, because EmptySet acts as a reactant. Nicolas Le Novere

Initial amount 0 µmol

This species takes part in four reactions (as a reactant in rM, rTL and as a product in rmRNAd, rVd), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{EmptySet} = 0 \tag{22}$$

7.2 Species M

Name PER mRNA

Notes Initial condition changed from amount to concentration as per article. Bruce Shapiro

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

This species takes part in three reactions (as a reactant in rmRNAd and as a product in rM and as a modifier in rTL).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{M} = v_1 - v_9 \tag{23}$$

7.3 Species P0

Name unphosphorylated PER

Notes Initial condition changed from amount to concentration as per article. Bruce Shapiro

Initial concentration $0.25\ \mu\mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in three reactions (as a reactant in rP01 and as a product in rTL, rP10).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{P0} = v_2 + v_4 - v_3 \tag{24}$$

7.4 Species P1

Name monophosphorylated PER

Notes Initial condition changed from amount to concentration as per article. Bruce Shapiro

Initial concentration $0.25\ \mu\mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in four reactions (as a reactant in rP10, rP12 and as a product in rP01, rP21).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{P1} = v_3 + v_6 - v_4 - v_5 \tag{25}$$

7.5 Species P2

Name biphosphorylated PER

Notes Initial condition changed from amount to concentration as per article. Bruce Shapiro

Initial concentration $0.25\ \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in five reactions (as a reactant in rP21, rP2n, rVd and as a product in rP12, rPn2).

$$\frac{\text{d}}{\text{d}t}\text{P2} = v_5 + v_8 - v_6 - v_7 - v_{10} \tag{26}$$

7.6 Species Pn

Name nuclear PER

Notes Initial condition changed from amount to concentration as per article. Bruce Shapiro

Initial concentration $0.25\ \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in three reactions (as a reactant in rPn2 and as a product in rP2n and as a modifier in rM).

$$\frac{\text{d}}{\text{d}t}\text{Pn} = v_7 - v_8 \tag{27}$$

7.7 Species Pt

Name total PER

Notes Initial condition changed from amount to concentration as per article. Bruce Shapiro

initial concentration for Pt is not used becuase Pt is determined by an Assigment Rule

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

Involved in rule Pt

One rule which determines this species' quantity.

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