SBML Model Report

Model name: “Leloup1998_CircClock_LD”

May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 1 format. This model was created by Lukas Endler[1] at May eighth 2008 at 10:48 a. m. and last time modified at April eighth 2016 at 3:38 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	2
species types	0	species	12
events	0	constraints	0
reactions	26	function definitions	0
global parameters	6	unit definitions	7
rules	3	initial assignments	0

Model Notes

Leloup and Goldbeter, 1998

This model was created after the article by Leloup and Goldbeter, *J Biol Rhythms* 1998, Vol:13(1),pp70-87, pubmedID: 9486845

> A Model for Circadian Rhythms in *Drosophila* Incorporating the Formation of a Complex between the PER and TIM Proteins

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The parameters and initial concentrations are taken to reproduce figs. 4 D,E,F in the publication. For a simulation without light dependent degradation of TIM_pp, change the the parameter v_dT_fac to 1.
The light/dark phases length can be set using the parameter l_d .

To cite BioModels Database, please use: Li C, Donizelli M, Rodriguez N, Dharuri H, Endler L, Chelliah V, Li L, He E, Henry A, Stefan MI, Snoep JL, Hucka M, Le Novre N, Laibe C (2010) BioModels Database: An enhanced, curated and annotated resource for published quantitative kinetic models. BMC Syst Biol., 4:92.

2 Unit Definitions

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

2.1 Unit `substance`

Name nanomolar

Definition nmol

2.2 Unit `nM`

Name nanomoleperlitre

Definition $\mathrm{nmol} \cdot \mathrm{l}^{-1}$

2.3 Unit `time`

Name hours

Definition 3.6 ks

2.4 Unit `nMph`

Name nanoMperHour

Definition $(3.6\,\mathrm{ks})^{-1} \cdot \mathrm{nmol} \cdot \mathrm{l}^{-1}$

2.5 Unit perh

Name perhour

Definition $(3.6\,\mathrm{ks})^{-1}$

2.6 Unit pnMph

Name pernMperHour

Definition $(3.6\,\mathrm{ks})^{-1} \cdot \mathrm{nmol}^{-1} \cdot \mathrm{l}$

2.7 Unit nmph

Name nanomolperhour

Definition $\mathrm{nmol} \cdot (3.6\,\mathrm{ks})^{-1}$

2.8 Unit volume

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

Definition l

2.9 Unit area

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

Definition m^2

2.10 Unit length

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

Definition m

3 Compartments

This model contains two compartments.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
nucleus			3	1		☑	
cytoplasm	cytoplasm		3	1		☑	

3.1 Compartment `nucleus`

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

3.2 Compartment `cytoplasm`

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

Name cytoplasm

4 Species

This model contains twelve species. The boundary condition of two of these species is set to `true` so that these species' amount cannot be changed by any reaction. Section 8 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
M_T	tim mRNA	cytoplasm	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
M_P	per mRNA	cytoplasm	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
T0	TIM	cytoplasm	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
T1	TIM-p	cytoplasm	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
T2	TIM-pp	cytoplasm	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
P0	PER	cytoplasm	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
P1	PER-p	cytoplasm	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
P2	PER-pp	cytoplasm	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
C	PER_TIM complex cytoplasm	cytoplasm	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
CN	PER_TIM complex nuclear	nucleus	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Tt	total TIM	cytoplasm	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	☑
Pt	total PER	cytoplasm	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	☑

5 Parameters

This model contains six global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
n	transkr_rep_hill-_coefficient		4.00	dimensionless	☑
kd	degradation_rate		0.01	$(3.6\,\mathrm{ks})^{-1}$	☑
v_dT	T2_lightdecay_rate		2.00	$(3.6\,\mathrm{ks})^{-1} \cdot \mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟
l_d	light_dark_period		12.00	3.6 ks	☑
v_dT_fac	v_dT_fold_incr-_during_light		2.00	dimensionless	☑
v_dT_dark	v_dT_value-_darkness		2.00	$(3.6\,\mathrm{ks})^{-1} \cdot \mathrm{nmol} \cdot \mathrm{l}^{-1}$	☑

6 Rules

This is an overview of three rules.

6.1 Rule Tt

Rule Tt is an assignment rule for species Tt:

$$\mathrm{Tt} = [\mathrm{T0}] + [\mathrm{T1}] + [\mathrm{T2}] + [\mathrm{C}] + \frac{[\mathrm{CN}] \cdot \mathrm{vol}\,(\mathrm{nucleus})}{\mathrm{vol}\,(\mathrm{cytoplasm})} \tag{1}$$

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

6.2 Rule Pt

Rule Pt is an assignment rule for species Pt:

$$\mathrm{Pt} = [\mathrm{P0}] + [\mathrm{P1}] + [\mathrm{P2}] + [\mathrm{C}] + \frac{[\mathrm{CN}] \cdot \mathrm{vol}\,(\mathrm{nucleus})}{\mathrm{vol}\,(\mathrm{cytoplasm})} \tag{2}$$

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

6.3 Rule v_dT

Rule v_dT is an assignment rule for parameter v_dT:

$$\mathrm{v\_dT} = \left(1 + (\mathrm{v\_dT\_fac} - 1) \cdot \left\lceil \sin\left(\frac{\mathrm{time}}{\mathrm{l\_d}} \cdot \pi\right) \cdot 0.9 \right\rceil\right) \cdot \mathrm{v\_dT\_dark} \tag{3}$$

7 Reactions

This model contains 26 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	per_trans	per transkription	$\emptyset \xrightarrow{\text{CN}} \text{M\_P}$	
2	tim_trans	tim transkription	$\emptyset \xrightarrow{\text{CN}} \text{M\_T}$	
3	M_T_decay	tim mRNA decay	$\text{M\_T} \longrightarrow \emptyset$	
4	M_P_decay	per mRNA decay	$\text{M\_P} \longrightarrow \emptyset$	
5	PER_transl	PER tranlation	$\emptyset \xrightarrow{\text{M\_P}} \text{P0}$	
6	TIM_transl	TIM translation	$\emptyset \xrightarrow{\text{M\_T}} \text{T0}$	
7	P0_decay	PER decay	$\text{P0} \longrightarrow \emptyset$	
8	P1_decay	PER-p decay	$\text{P1} \longrightarrow \emptyset$	
9	P2_decay	PER-pp decay	$\text{P2} \longrightarrow \emptyset$	
10	T0_decay	TIM decay	$\text{T0} \longrightarrow \emptyset$	
11	T1_decay	TIM-p decay	$\text{T1} \longrightarrow \emptyset$	
12	T2_decay	TIM-pp decay	$\text{T2} \longrightarrow \emptyset$	
13	C_form	Per_TIM complex formation	$\text{P2} + \text{T2} \longrightarrow \text{C}$	
14	C_decay	cytopl. PER_TIM compl. decay	$\text{C} \longrightarrow \emptyset$	
15	CN_decay	nuclear PER_TIM compl. decay	$\text{CN} \longrightarrow \emptyset$	
16	C_transp	PER_TIM complex shuttling	$\text{C} \rightleftharpoons \text{CN}$	
17	P_pho	PER phosphorylation	$\text{P0} \longrightarrow \text{P1}$	
18	P1_pho	PER-p phosphorylation	$\text{P1} \longrightarrow \text{P2}$	
19	P1_depho	PER-p dephosphorylation	$\text{P1} \longrightarrow \text{P0}$	
20	P2_depho	PER-pp dephosphorylation	$\text{P2} \longrightarrow \text{P1}$	
21	T_pho	TIM phosphorylation	$\text{T0} \longrightarrow \text{T1}$	

№	Id	Name	Reaction Equation	SBO
22	T1_pho	TIM-p phosphorylation	T1 ⟶ T2	
23	T1_depho	TIM-p dephosphorylation	T1 ⟶ T0	
24	T2_depho	TIM-pp dephosphorylation	T2 ⟶ T1	
25	T2_light_deact	TIM-pp light deactivation	T2 ⟶ ∅	
26	P2_light_deact	PER-pp light deactivation	P2 ⟶ ∅	

7.1 Reaction per_trans

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

Name per transkription

Reaction equation

$$\emptyset \xrightarrow{\mathrm{CN}} \mathrm{M\_P} \tag{4}$$

Modifier

Table 6: Properties of each modifier.

Id	Name	SBO
CN	PER_TIM complex nuclear	

Product

Table 7: Properties of each product.

Id	Name	SBO
M_P	per mRNA	

Kinetic Law

Derived unit $9.99999999999994 \cdot 10^{-10}\ \mathrm{mol} \cdot (3.6\ \mathrm{ks})^{-1}$

$$v_1 = \frac{\mathrm{v\_sP} \cdot \mathrm{Ki\_P^n}}{\mathrm{Ki\_P^n} + [\mathrm{CN}]^n} \tag{5}$$

Table 8: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
v_sP	per_max_transkr-_rate		0.8	$\mathrm{nmol} \cdot (3.6\ \mathrm{ks})^{-1}$	☑
Ki_P	per_inh_konstant		1.0	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	☑

7.2 Reaction tim_trans

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

Name tim transkription

Reaction equation

$$\emptyset \xrightarrow{\text{CN}} \text{M\_T} \tag{6}$$

Modifier

Table 9: Properties of each modifier.

Id	Name	SBO
CN	PER_TIM complex nuclear	

Product

Table 10: Properties of each product.

Id	Name	SBO
M_T	tim mRNA	

Kinetic Law

Derived unit $9.99999999999994 \cdot 10^{-10}\ \text{mol} \cdot (3.6\ \text{ks})^{-1}$

$$v_2 = \frac{\text{v\_sT} \cdot \text{Ki\_T}^{\text{n}}}{\text{Ki\_T}^{\text{n}} + [\text{CN}]^{\text{n}}} \tag{7}$$

Table 11: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
v_sT	tim_max_transkr-_rate		1.0	$\text{nmol} \cdot (3.6\ \text{ks})^{-1}$	☑
Ki_T	tim_inh_konstant		1.0	$\text{nmol} \cdot 1^{-1}$	☑

7.3 Reaction M_T_decay

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

Name tim mRNA decay

Reaction equation

$$\text{M\_T} \longrightarrow \emptyset \tag{8}$$

Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
M_T	tim mRNA	

Kinetic Law

Derived unit $(3.6\,\text{ks})^{-1} \cdot \text{nmol}$

$$v_3 = \left(\frac{\text{v\_mT}}{\text{K\_mT} + [\text{M\_T}]} + \text{kd} \right) \cdot [\text{M\_T}] \cdot \text{vol}\,(\text{cytoplasm}) \tag{9}$$

Table 13: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
v_mT	M_T_mm_decay		0.7	$(3.6\,\text{ks})^{-1} \cdot \text{nmol} \cdot \text{l}^{-1}$	☑
K_mT	decay_KM_T		0.2	$\text{nmol} \cdot \text{l}^{-1}$	☑

7.4 Reaction M_P_decay

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

Name per mRNA decay

Reaction equation

$$\text{M\_P} \longrightarrow \emptyset \tag{10}$$

Reactant

Table 14: Properties of each reactant.

Id	Name	SBO
M_P	per mRNA	

Kinetic Law

Derived unit $(3.6\,\mathrm{ks})^{-1} \cdot \mathrm{nmol}$

$$v_4 = \left(\frac{\mathrm{v\_mP}}{\mathrm{K\_mP} + [\mathrm{M\_P}]} + \mathrm{kd} \right) \cdot [\mathrm{M\_P}] \cdot \mathrm{vol}\,(\mathrm{cytoplasm}) \tag{11}$$

Table 15: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
v_mP	max_M_P_decay-_rate		0.8	$(3.6\,\mathrm{ks})^{-1} \cdot \mathrm{nmol} \cdot \mathrm{l}^{-1}$	☑
K_mP	M_P_decay_Km		0.2	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	☑

7.5 Reaction PER_transl

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

Name PER tranlation

Reaction equation

$$\emptyset \xrightarrow{\mathrm{M\_P}} \mathrm{P0} \tag{12}$$

Modifier

Table 16: Properties of each modifier.

Id	Name	SBO
M_P	per mRNA	

Product

Table 17: Properties of each product.

Id	Name	SBO
P0	PER	

Kinetic Law

Derived unit $(3.6\,\mathrm{ks})^{-1} \cdot \mathrm{nmol}$

$$v_5 = \text{k\_sP} \cdot [\text{M\_P}] \cdot \text{vol}\,(\text{cytoplasm}) \tag{13}$$

Table 18: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k_sP	PER_translation-_rate		0.9	$(3.6\,\text{ks})^{-1}$	☑

7.6 Reaction TIM_transl

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

Name TIM translation

Reaction equation

$$\emptyset \xrightarrow{\text{M\_T}} \text{T0} \tag{14}$$

Modifier

Table 19: Properties of each modifier.

Id	Name	SBO
M_T	tim mRNA	

Product

Table 20: Properties of each product.

Id	Name	SBO
T0	TIM	

Kinetic Law

Derived unit $(3.6\,\text{ks})^{-1} \cdot \text{nmol}$

$$v_6 = \text{k\_sT} \cdot [\text{M\_T}] \cdot \text{vol}\,(\text{cytoplasm}) \tag{15}$$

Table 21: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k_sT	TIM_translation-_rate		0.9	$(3.6\,\mathrm{ks})^{-1}$	☑

7.7 Reaction P0_decay

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

Name PER decay

Reaction equation

$$\mathrm{P0} \longrightarrow \emptyset \tag{16}$$

Reactant

Table 22: Properties of each reactant.

Id	Name	SBO
P0	PER	

Kinetic Law

Derived unit $(3.6\,\mathrm{ks})^{-1} \cdot \mathrm{nmol}$

$$v_7 = \mathrm{kd} \cdot [\mathrm{P0}] \cdot \mathrm{vol}\,(\mathrm{cytoplasm}) \tag{17}$$

7.8 Reaction P1_decay

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

Name PER-p decay

Reaction equation

$$\mathrm{P1} \longrightarrow \emptyset \tag{18}$$

Reactant

Table 23: Properties of each reactant.

Id	Name	SBO
P1	PER-p	

Kinetic Law

Derived unit $(3.6\,\mathrm{ks})^{-1} \cdot \mathrm{nmol}$

$$v_8 = \mathrm{kd} \cdot [\mathrm{P1}] \cdot \mathrm{vol}\,(\mathrm{cytoplasm}) \tag{19}$$

7.9 Reaction P2_decay

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

Name PER-pp decay

Reaction equation

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

Reactant

Table 24: Properties of each reactant.

Id	Name	SBO
P2	PER-pp	

Kinetic Law

Derived unit $(3.6\,\mathrm{ks})^{-1} \cdot \mathrm{nmol}$

$$v_9 = \mathrm{kd} \cdot [\mathrm{P2}] \cdot \mathrm{vol}\,(\mathrm{cytoplasm}) \tag{21}$$

7.10 Reaction T0_decay

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

Name TIM decay

Reaction equation

$$\mathrm{T0} \longrightarrow \emptyset \tag{22}$$

Reactant

Table 25: Properties of each reactant.

Id	Name	SBO
T0	TIM	

Kinetic Law

Derived unit $(3.6\,\mathrm{ks})^{-1} \cdot \mathrm{nmol}$

$$v_{10} = \mathrm{kd} \cdot [\mathrm{T0}] \cdot \mathrm{vol}\,(\mathrm{cytoplasm}) \tag{23}$$

7.11 Reaction T1_decay

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

Name TIM-p decay

Reaction equation

$$\mathrm{T1} \longrightarrow \emptyset \tag{24}$$

Reactant

Table 26: Properties of each reactant.

Id	Name	SBO
T1	TIM-p	

Kinetic Law

Derived unit $(3.6\,\mathrm{ks})^{-1} \cdot \mathrm{nmol}$

$$v_{11} = \mathrm{kd} \cdot [\mathrm{T1}] \cdot \mathrm{vol}\,(\mathrm{cytoplasm}) \tag{25}$$

7.12 Reaction T2_decay

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

Name TIM-pp decay

Reaction equation

$$\mathrm{T2} \longrightarrow \emptyset \tag{26}$$

Reactant

Table 27: Properties of each reactant.

Id	Name	SBO
T2	TIM-pp	

Kinetic Law

Derived unit $(3.6\,\mathrm{ks})^{-1} \cdot \mathrm{nmol}$

$$v_{12} = \mathrm{kd} \cdot [\mathrm{T2}] \cdot \mathrm{vol}\,(\mathrm{cytoplasm}) \tag{27}$$

7.13 Reaction C_form

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

Name Per_TIM complex formation

Reaction equation

$$\mathrm{P2} + \mathrm{T2} \longrightarrow \mathrm{C} \tag{28}$$

Reactants

Table 28: Properties of each reactant.

Id	Name	SBO
P2	PER-pp	
T2	TIM-pp	

Product

Table 29: Properties of each product.

Id	Name	SBO
C	PER_TIM complex cytoplasm	

Kinetic Law

Derived unit $(3.6\,\mathrm{ks})^{-1} \cdot \mathrm{nmol}$

$$v_{13} = (\mathrm{k3} \cdot [\mathrm{T2}] \cdot [\mathrm{P2}] - \mathrm{k4} \cdot [\mathrm{C}]) \cdot \mathrm{vol}\,(\mathrm{cytoplasm}) \tag{29}$$

Table 30: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k3	T_P_ass_rate		1.2	$(3.6\,\mathrm{ks})^{-1} \cdot \mathrm{nmol}^{-1} \cdot 1$	☑
k4	C_diss_rate		0.6	$(3.6\,\mathrm{ks})^{-1}$	☑

7.14 Reaction C_decay

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

Name cytopl. PER_TIM compl. decay

Reaction equation

$$\mathrm{C} \longrightarrow \emptyset \tag{30}$$

Reactant

Table 31: Properties of each reactant.

Id	Name	SBO
C	PER_TIM complex cytoplasm	

Kinetic Law

Derived unit $(3.6\,\mathrm{ks})^{-1} \cdot \mathrm{nmol}$

$$v_{14} = \mathrm{kd\_C} \cdot [\mathrm{C}] \cdot \mathrm{vol}\,(\mathrm{cytoplasm}) \tag{31}$$

Table 32: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
kd_C	C_decay_rate		0.01	$(3.6\,\mathrm{ks})^{-1}$	☑

7.15 Reaction CN_decay

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

Name nuclear PER_TIM compl. decay

Reaction equation

$$\mathrm{CN} \longrightarrow \emptyset \tag{32}$$

Reactant

Table 33: Properties of each reactant.

Id	Name	SBO
CN	PER_TIM complex nuclear	

Kinetic Law

Derived unit $(3.6\,\mathrm{ks})^{-1} \cdot \mathrm{nmol}$

$$v_{15} = \mathrm{kd\_CN} \cdot [\mathrm{CN}] \cdot \mathrm{vol}\,(\mathrm{nucleus}) \tag{33}$$

Table 34: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
kd_CN	CN_decay_rate		0.01	$(3.6\,\mathrm{ks})^{-1}$	☑

7.16 Reaction C_transp

This is a reversible reaction of one reactant forming one product.

Name PER_TIM complex shuttling

Reaction equation

$$\mathrm{C} \rightleftharpoons \mathrm{CN} \tag{34}$$

Reactant

Table 35: Properties of each reactant.

Id	Name	SBO
C	PER_TIM complex cytoplasm	

Product

Table 36: Properties of each product.

Id	Name	SBO
CN	PER_TIM complex nuclear	

Kinetic Law

Derived unit $(3.6\,\mathrm{ks})^{-1} \cdot \mathrm{nmol}$

$$v_{16} = \mathrm{k1} \cdot [\mathrm{C}] \cdot \mathrm{vol}\,(\mathrm{cytoplasm}) - \mathrm{k2} \cdot [\mathrm{CN}] \cdot \mathrm{vol}\,(\mathrm{nucleus}) \tag{35}$$

Table 37: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1	C_import_rate		1.2	$(3.6\,\mathrm{ks})^{-1}$	☑
k2	C_export_rate		0.2	$(3.6\,\mathrm{ks})^{-1}$	☑

7.17 Reaction P_pho

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

Name PER phosphorylation

Reaction equation

$$\mathrm{P0} \longrightarrow \mathrm{P1} \tag{36}$$

Reactant

Table 38: Properties of each reactant.

Id	Name	SBO
P0	PER	

Product

Table 39: Properties of each product.

Id	Name	SBO
P1	PER-p	

Kinetic Law

Derived unit $(3.6\,\mathrm{ks})^{-1} \cdot 9.999999999999998 \cdot 10^{-10}\,\mathrm{mol}$

$$v_{17} = \frac{\mathrm{V\_1P} \cdot [\mathrm{P0}]}{\mathrm{K\_1P} + [\mathrm{P0}]} \cdot \mathrm{vol}\,(\mathrm{cytoplasm}) \tag{37}$$

Table 40: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V_1P	P0_phos_rate		8.0	$(3.6\,\mathrm{ks})^{-1} \cdot \mathrm{nmol} \cdot \mathrm{l}^{-1}$	☑
K_1P	P0_kinase_KM		2.0	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	☑

7.18 Reaction P1_pho

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

Name PER-p phosphorylation

Reaction equation

$$\mathrm{P1} \longrightarrow \mathrm{P2} \tag{38}$$

Reactant

Table 41: Properties of each reactant.

Id	Name	SBO
P1	PER-p	

Product

Table 42: Properties of each product.

Id	Name	SBO
P2	PER-pp	

Kinetic Law

Derived unit $(3.6\,\mathrm{ks})^{-1} \cdot 9.999999999999998 \cdot 10^{-10}\,\mathrm{mol}$

$$v_{18} = \frac{\mathrm{V\_3P} \cdot [\mathrm{P1}]}{\mathrm{K\_3P} + [\mathrm{P1}]} \cdot \mathrm{vol}\,(\mathrm{cytoplasm}) \tag{39}$$

Table 43: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V_3P	P1_phosph_rate		8.0	$(3.6\,\mathrm{ks})^{-1} \cdot \mathrm{nmol} \cdot \mathrm{l}^{-1}$	☑
K_3P	P1_kinase_KM		2.0	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	☑

7.19 Reaction P1_depho

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

Name PER-p dephosphorylation

Reaction equation

$$\mathrm{P1} \longrightarrow \mathrm{P0} \tag{40}$$

Reactant

Table 44: Properties of each reactant.

Id	Name	SBO
P1	PER-p	

Product

Table 45: Properties of each product.

Id	Name	SBO
P0	PER	

Kinetic Law

Derived unit $(3.6\,\mathrm{ks})^{-1} \cdot 9.999999999999998 \cdot 10^{-10}\,\mathrm{mol}$

$$v_{19} = \frac{\mathrm{V\_2P} \cdot [\mathrm{P1}]}{\mathrm{K\_2P} + [\mathrm{P1}]} \cdot \mathrm{vol}\,(\mathrm{cytoplasm}) \tag{41}$$

Table 46: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
K_2P	P1_phosphatase-_KM		2.0	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	☑
V_2P	P1_dephos_rate		1.0	$(3.6\,\mathrm{ks})^{-1} \cdot \mathrm{nmol} \cdot \mathrm{l}^{-1}$	☑

7.20 Reaction P2_depho

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

Name PER-pp dephosphorylation

Reaction equation

$$\mathrm{P2} \longrightarrow \mathrm{P1} \tag{42}$$

Reactant

Table 47: Properties of each reactant.

Id	Name	SBO
P2	PER-pp	

Product

Table 48: Properties of each product.

Id	Name	SBO
P1	PER-p	

Kinetic Law

Derived unit $(3.6\,\mathrm{ks})^{-1} \cdot 9.999999999999998 \cdot 10^{-10}\,\mathrm{mol}$

$$v_{20} = \frac{\mathrm{V\_4P} \cdot [\mathrm{P2}]}{\mathrm{K\_4P} + [\mathrm{P2}]} \cdot \mathrm{vol}\,(\mathrm{cytoplasm}) \tag{43}$$

Table 49: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V_4P	P2_dephos_rate		1.0	$(3.6\,\mathrm{ks})^{-1} \cdot \mathrm{nmol} \cdot \mathrm{l}^{-1}$	☑
K_4P	P2_phosphatase-_KM		2.0	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	☑

7.21 Reaction T_pho

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

Name TIM phosphorylation

Reaction equation

$$\mathrm{T0} \longrightarrow \mathrm{T1} \tag{44}$$

Reactant

Table 50: Properties of each reactant.

Id	Name	SBO
T0	TIM	

Product

Table 51: Properties of each product.

Id	Name	SBO
T1	TIM-p	

Kinetic Law

Derived unit $(3.6\,\mathrm{ks})^{-1} \cdot 9.999999999999998 \cdot 10^{-10}\,\mathrm{mol}$

$$v_{21} = \frac{\mathrm{V\_1T} \cdot [\mathrm{T0}]}{\mathrm{K\_1T} + [\mathrm{T0}]} \cdot \mathrm{vol}\,(\mathrm{cytoplasm}) \tag{45}$$

Table 52: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V_1T	T0_phos_rate		8.0	$(3.6\,\mathrm{ks})^{-1} \cdot \mathrm{nmol} \cdot \mathrm{l}^{-1}$	☑
K_1T	T0_kinase_KM		2.0	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	☑

7.22 Reaction T1_pho

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

Name TIM-p phosphorylation

Reaction equation

$$\mathrm{T1} \longrightarrow \mathrm{T2} \tag{46}$$

Reactant

Table 53: Properties of each reactant.

Id	Name	SBO
T1	TIM-p	

Product

Table 54: Properties of each product.

Id	Name	SBO
T2	TIM-pp	

Kinetic Law

Derived unit $(3.6\,\mathrm{ks})^{-1} \cdot 9.999999999999998 \cdot 10^{-10}\,\mathrm{mol}$

$$v_{22} = \frac{\mathrm{V\_3T} \cdot [\mathrm{T1}]}{\mathrm{K\_3T} + [\mathrm{T1}]} \cdot \mathrm{vol}\,(\mathrm{cytoplasm}) \tag{47}$$

Table 55: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V_3T	T1_phosph_rate		8.0	$(3.6\,\mathrm{ks})^{-1} \cdot \mathrm{nmol} \cdot \mathrm{l}^{-1}$	☑
K_3T	T1_kinase_KM		2.0	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	☑

7.23 Reaction T1_depho

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

Name TIM-p dephosphorylation

Reaction equation

$$\mathrm{T1} \longrightarrow \mathrm{T0} \tag{48}$$

Reactant

Table 56: Properties of each reactant.

Id	Name	SBO
T1	TIM-p	

Product

Table 57: Properties of each product.

Id	Name	SBO
T0	TIM	

Kinetic Law

Derived unit $(3.6\,\mathrm{ks})^{-1} \cdot 9.999999999999998 \cdot 10^{-10}\,\mathrm{mol}$

$$v_{23} = \frac{\mathrm{V\_2T} \cdot [\mathrm{T1}]}{\mathrm{K\_2T} + [\mathrm{T1}]} \cdot \mathrm{vol}\,(\mathrm{cytoplasm}) \tag{49}$$

Table 58: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
K_2T	T1_phosphatase-_KM		2.0	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	☑
V_2T	T1_dephos_rate		1.0	$(3.6\,\mathrm{ks})^{-1} \cdot \mathrm{nmol} \cdot \mathrm{l}^{-1}$	☑

7.24 Reaction T2_depho

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

Name TIM-pp dephosphorylation

Reaction equation

$$\mathrm{T2} \longrightarrow \mathrm{T1} \tag{50}$$

Reactant

Table 59: Properties of each reactant.

Id	Name	SBO
T2	TIM-pp	

Product

Table 60: Properties of each product.

Id	Name	SBO
T1	TIM-p	

Kinetic Law

Derived unit $(3.6\,\mathrm{ks})^{-1} \cdot 9.999999999999998 \cdot 10^{-10}\,\mathrm{mol}$

$$v_{24} = \frac{\mathrm{V\_4T} \cdot [\mathrm{T2}]}{\mathrm{K\_4T} + [\mathrm{T2}]} \cdot \mathrm{vol}\,(\mathrm{cytoplasm}) \tag{51}$$

Table 61: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V_4T	T2_dephos_rate		1.0	$(3.6\,\mathrm{ks})^{-1} \cdot \mathrm{nmol} \cdot \mathrm{l}^{-1}$	☑
K_4T	T2_phosphatase-_KM		2.0	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	☑

7.25 Reaction T2_light_deact

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

Name TIM-pp light deactivation

Reaction equation

$$\mathrm{T2} \longrightarrow \emptyset \tag{52}$$

Reactant

Table 62: Properties of each reactant.

Id	Name	SBO
T2	TIM-pp	

Kinetic Law

Derived unit $(3.6\,\mathrm{ks})^{-1} \cdot 9.999999999999998 \cdot 10^{-10}\,\mathrm{mol}$

$$v_{25} = \frac{\text{v\_dT} \cdot [\text{T2}]}{\text{K\_dT} + [\text{T2}]} \cdot \text{vol}\,(\text{cytoplasm}) \tag{53}$$

Table 63: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
K_dT	T2_light_deact_KM		0.2	$\text{nmol} \cdot \text{l}^{-1}$	☑

7.26 Reaction P2_light_deact

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

Name PER-pp light deactivation

Reaction equation

$$\text{P2} \longrightarrow \emptyset \tag{54}$$

Reactant

Table 64: Properties of each reactant.

Id	Name	SBO
P2	PER-pp	

Kinetic Law

Derived unit $(3.6\,\text{ks})^{-1} \cdot 9.999999999999998 \cdot 10^{-10}\,\text{mol}$

$$v_{26} = \frac{\text{v\_dP} \cdot [\text{P2}]}{\text{K\_dP} + [\text{P2}]} \cdot \text{vol}\,(\text{cytoplasm}) \tag{55}$$

Table 65: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
v_dP	P2_light-_deactivation_rate		2.0	$(3.6\,\text{ks})^{-1} \cdot \text{nmol} \cdot \text{l}^{-1}$	☑
K_dP	P2_light-_deactivation_KM		0.2	$\text{nmol} \cdot \text{l}^{-1}$	☑

8 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.

8.1 Species M_T

Name tim mRNA

Initial concentration $1.41\ \mathrm{nmol}\cdot\mathrm{l}^{-1}$

This species takes part in three reactions (as a reactant in M_T_decay and as a product in tim_trans and as a modifier in TIM_transl).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{M\_T} = v_2 - v_3 \tag{56}$$

8.2 Species M_P

Name per mRNA

Initial concentration $0.09\ \mathrm{nmol}\cdot\mathrm{l}^{-1}$

This species takes part in three reactions (as a reactant in M_P_decay and as a product in per_trans and as a modifier in PER_transl).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{M\_P} = v_1 - v_4 \tag{57}$$

8.3 Species T0

Name TIM

Initial concentration $0.54\ \mathrm{nmol}\cdot\mathrm{l}^{-1}$

This species takes part in four reactions (as a reactant in T0_decay, T_pho and as a product in TIM_transl, T1_depho).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{T0} = v_6 + v_{23} - v_{10} - v_{21} \tag{58}$$

8.4 Species T1

Name TIM-p

Initial concentration $0.79\ \mathrm{nmol}\cdot\mathrm{l}^{-1}$

This species takes part in five reactions (as a reactant in T1_decay, T1_pho, T1_depho and as a product in T_pho, T2_depho).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{T1} = v_{21} + v_{24} - v_{11} - v_{22} - v_{23} \tag{59}$$

8.5 Species T2

Name TIM-pp

Initial concentration $4.65\ \mathrm{nmol}\cdot\mathrm{l}^{-1}$

This species takes part in five reactions (as a reactant in T2_decay, C_form, T2_depho, T2-_light_deact and as a product in T1_pho).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{T2} = v_{22} - v_{12} - v_{13} - v_{24} - v_{25} \tag{60}$$

8.6 Species P0

Name PER

Initial concentration $0.02\ \mathrm{nmol}\cdot\mathrm{l}^{-1}$

This species takes part in four reactions (as a reactant in P0_decay, P_pho and as a product in PER_transl, P1_depho).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{P0} = v_5 + v_{19} - v_7 - v_{17} \tag{61}$$

8.7 Species P1

Name PER-p

Initial concentration $0.02\ \mathrm{nmol}\cdot\mathrm{l}^{-1}$

This species takes part in five reactions (as a reactant in P1_decay, P1_pho, P1_depho and as a product in P_pho, P2_depho).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{P1} = v_{17} + v_{20} - v_8 - v_{18} - v_{19} \tag{62}$$

8.8 Species P2

Name PER-pp

Initial concentration $0.01\ \mathrm{nmol}\cdot\mathrm{l}^{-1}$

This species takes part in five reactions (as a reactant in P2_decay, C_form, P2_depho, P2-_light_deact and as a product in P1_pho).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{P2} = v_{18} - v_9 - v_{13} - v_{20} - v_{26} \tag{63}$$

8.9 Species C

Name PER_TIM complex cytoplasm

Initial concentration $0.18\ \mathrm{nmol}\cdot\mathrm{l}^{-1}$

This species takes part in three reactions (as a reactant in C_decay, C_transp and as a product in C_form).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{C} = v_{13} - v_{14} - v_{16} \tag{64}$$

8.10 Species CN

Name PER_TIM complex nuclear

Initial concentration $1.2\ \mathrm{nmol}\cdot\mathrm{l}^{-1}$

This species takes part in four reactions (as a reactant in CN_decay and as a product in C_transp and as a modifier in per_trans, tim_trans).

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

8.11 Species Tt

Name total TIM

Involved in rule Tt

One rule determines the species' quantity.

8.12 Species Pt

Name total PER

Involved in rule Pt

One rule determines the species' quantity.

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