SBML Model Report

Model name: "Hong2009_CircadianClock"

May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 3 format. This model was created by the following three authors: Vijayalakshmi Chelliah[1], Christian Hong[2] and Judit Zamborszky[3] at April third 2009 at 11:51 a. m. and last time modified at February 25th 2015 at 1:15 p. m. Table 1 gives 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	6
events	0	constraints	0
reactions	17	function definitions	6
global parameters	18	unit definitions	0
rules	1	initial assignments	0

Model Notes

This a model from the article:
Minimum criteria for DNA damage-induced phase advances in circadian rhythms.
Hong CI, Zmborszky J, Csiksz-Nagy A. PLoS Comput Biol. 2009 May;5(5):e1000384. 19424508,
Abstract:

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Robust oscillatory behaviors are common features of circadian and cell cycle rhythms. These cyclic processes, however, behave distinctively in terms of their periods and phases in response to external influences such as light, temperature, nutrients, etc. Nevertheless, several links have been found between these two oscillators. Cell division cycles gated by the circadian clock have been observed since the late 1950s. On the other hand, ionizing radiation (IR) treatments cause cells to undergo a DNA damage response, which leads to phase shifts (mostly advances) in circadian rhythms. Circadian gating of the cell cycle can be attributed to the cell cycle inhibitor kinase Wee1 (which is regulated by the heterodimeric circadian clock transcription factor, BMAL1/CLK), and possibly in conjunction with other cell cycle components that are known to be regulated by the circadian clock (i.e., c-Myc and cyclin D1). It has also been shown that DNA damage-induced activation of the cell cycle regulator, Chk2, leads to phosphorylation and destruction of a circadian clock component (i.e., PER1 in Mus or FRQ in Neurospora crassa). However, the molecular mechanism underlying how DNA damage causes predominantly phase advances in the circadian clock remains unknown. In order to address this question, we employ mathematical modeling to simulate different phase response curves (PRCs) from either dexamethasone (Dex) or IR treatment experiments. Dex is known to synchronize circadian rhythms in cell culture and may generate both phase advances and delays. We observe unique phase responses with minimum delays of the circadian clock upon DNA damage when two criteria are met: (1) existence of an autocatalytic positive feedback mechanism in addition to the time-delayed negative feedback loop in the clock system and (2) Chk2-dependent phosphorylation and degradation of PERs that are not bound to BMAL1/CLK.

The original xpp file of the model is available as a supplement of the article (Text S1).

2 Unit Definitions

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

2.1 Unit `substance`

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

Definition mol

2.2 Unit `volume`

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

Definition l

2.3 Unit `area`

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

Definition m^2

2.4 Unit `length`

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

Definition m

2.5 Unit `time`

Notes Second is the predefined SBML unit for `time`.

Definition s

3 Compartment

This model contains one compartment.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
`system`	system	0000290	3	1	litre	☑	

3.1 Compartment `system`

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

Name system

SBO:0000290 physical compartment

4 Species

This model contains six 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 9 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`	M	`system`	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☐
`TF`	TF	`system`	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☐
`CP`	CP	`system`	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☐
`CP2`	CP2	`system`	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☐
`IC`	IC	`system`	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☐
`CPtot`	CPtot	`system`	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☑

5 Parameters

This model contains 18 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Dex	Dex	0000196	0.000		☑
kms	kms		1.000		☑
n	n		2.000		☑
J	J		0.300		☑
kmd	kmd		0.100		☑
kcps	kcps		0.500		☑
kcpd	kcpd		0.525		☑
ka	ka		100.000		☑
kd	kd		0.010		☑
kp1	kp1		10.000		☑
Jp	Jp		0.050		☑
chk2	chk2		0.000		☑
kicd	kicd		0.010		☑
kcp2d	kcp2d		0.053		☑
kica	kica		20.000		☑
chk2c	chk2c		0.000		☑
kp2	kp2		0.100		☑
ICtot	TFtot		1.000		☑

6 Function definitions

This is an overview of six function definitions.

6.1 Function definition function_4_r1

Name function_4_r1

Arguments Dex, vol (system)

Mathematical Expression

$$\frac{\text{Dex}}{\text{vol}\,(\text{system})} \tag{1}$$

6.2 Function definition function_4_r8

Name function_4_r8

Arguments [CP], [CP2], [IC], Jp, kp1, vol (system)

Mathematical Expression

$$\frac{\frac{\mathrm{kp1}\cdot[\mathrm{CP}]}{\mathrm{Jp}+[\mathrm{CP}]+2\cdot[\mathrm{CP2}]+2\cdot[\mathrm{IC}]}}{\mathrm{vol}\,(\mathrm{system})} \tag{2}$$

6.3 Function definition function_4_r2

Name function_4_r2

Arguments J, [TF], kms, n, vol (system)

Mathematical Expression

$$\frac{\frac{\mathrm{kms}\cdot[\mathrm{TF}]^{\mathrm{n}}}{\mathrm{J}^{\mathrm{n}}+[\mathrm{TF}]^{\mathrm{n}}}}{\mathrm{vol}\,(\mathrm{system})} \tag{3}$$

6.4 Function definition function_4_r17

Name function_4_r17

Arguments [CP], [CP2], [IC], Jp, kp2, vol (system)

Mathematical Expression

$$\frac{\frac{\mathrm{kp2}\cdot[\mathrm{IC}]}{\mathrm{Jp}+[\mathrm{CP}]+2\cdot[\mathrm{CP2}]+2\cdot[\mathrm{IC}]}}{\mathrm{vol}\,(\mathrm{system})} \tag{4}$$

6.5 Function definition function_4_r13

Name function_4_r13

Arguments [CP], [CP2], [IC], Jp, kp2, vol (system)

Mathematical Expression

$$\frac{\frac{\mathrm{kp2}\cdot[\mathrm{CP2}]}{\mathrm{Jp}+[\mathrm{CP}]+2\cdot[\mathrm{CP2}]+2\cdot[\mathrm{IC}]}}{\mathrm{vol}\,(\mathrm{system})} \tag{5}$$

6.6 Function definition function_1

Name Rate Law for r4

Arguments kcps, [M]

Mathematical Expression

$$\mathrm{kcps}\cdot[\mathrm{M}] \tag{6}$$

7 Rule

This is an overview of one rule.

7.1 Rule `CPtot`

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

$$\text{CPtot} = [\text{CP}] + 2 \cdot [\text{CP2}] + 2 \cdot [\text{IC}] \tag{7}$$

8 Reactions

This model contains 17 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	r1	r1	$\emptyset \longrightarrow M$	
2	r2	r2	$\emptyset \xrightarrow{TF} M$	
3	r3	r3	$M \longrightarrow \emptyset$	
4	r4	r4	$\emptyset \xrightarrow{M} CP$	
5	r5	r5	$CP \longrightarrow \emptyset$	
6	r6	r6	$2\,CP \longrightarrow CP2$	
7	r7	r7	$CP2 \longrightarrow 2\,CP$	
8	r8	r8	$CP \xrightarrow{CP2,\ IC} \emptyset$	
9	r9	r9	$CP \longrightarrow \emptyset$	
10	r10	r10	$IC \longrightarrow CP2 + TF$	
11	r11	r11	$CP2 \longrightarrow \emptyset$	
12	r12	r12	$CP2 + TF \longrightarrow IC$	
13	r13	r13	$CP2 \xrightarrow{CP,\ IC} \emptyset$	
14	r14	r14	$CP2 \longrightarrow \emptyset$	
15	r15	r15	$IC \longrightarrow TF$	
16	r16	r16	$IC \longrightarrow TF$	
17	r17	r17	$IC \xrightarrow{CP2,\ CP} TF$	

8.1 Reaction r1

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

Name r1

Reaction equation

$$\emptyset \longrightarrow \mathrm{M} \tag{8}$$

Product

Table 6: Properties of each product.

Id	Name	SBO
M	M	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \mathrm{vol}\left(\mathrm{system}\right) \cdot \mathrm{function\_4\_r1}\left(\mathrm{Dex}, \mathrm{vol}\left(\mathrm{system}\right)\right) \tag{9}$$

$$\mathrm{function\_4\_r1}\left(\mathrm{Dex}, \mathrm{vol}\left(\mathrm{system}\right)\right) = \frac{\mathrm{Dex}}{\mathrm{vol}\left(\mathrm{system}\right)} \tag{10}$$

$$\mathrm{function\_4\_r1}\left(\mathrm{Dex}, \mathrm{vol}\left(\mathrm{system}\right)\right) = \frac{\mathrm{Dex}}{\mathrm{vol}\left(\mathrm{system}\right)} \tag{11}$$

8.2 Reaction r2

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

Name r2

Reaction equation

$$\emptyset \xrightarrow{\mathrm{TF}} \mathrm{M} \tag{12}$$

Modifier

Table 7: Properties of each modifier.

Id	Name	SBO
TF	TF	

Product

Table 8: Properties of each product.

Id	Name	SBO
M	M	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \mathrm{vol}\left(\mathrm{system}\right) \cdot \mathrm{function\_4\_r2}\left(\mathrm{J}, [\mathrm{TF}], \mathrm{kms}, \mathrm{n}, \mathrm{vol}\left(\mathrm{system}\right)\right) \tag{13}$$

$$\mathrm{function\_4\_r2}\left(\mathrm{J}, [\mathrm{TF}], \mathrm{kms}, \mathrm{n}, \mathrm{vol}\left(\mathrm{system}\right)\right) = \frac{\frac{\mathrm{kms} \cdot [\mathrm{TF}]^{\mathrm{n}}}{\mathrm{J}^{\mathrm{n}} + [\mathrm{TF}]^{\mathrm{n}}}}{\mathrm{vol}\left(\mathrm{system}\right)} \tag{14}$$

$$\mathrm{function\_4\_r2}\left(\mathrm{J}, [\mathrm{TF}], \mathrm{kms}, \mathrm{n}, \mathrm{vol}\left(\mathrm{system}\right)\right) = \frac{\frac{\mathrm{kms} \cdot [\mathrm{TF}]^{\mathrm{n}}}{\mathrm{J}^{\mathrm{n}} + [\mathrm{TF}]^{\mathrm{n}}}}{\mathrm{vol}\left(\mathrm{system}\right)} \tag{15}$$

8.3 Reaction r3

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

Name r3

Reaction equation

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

Reactant

Table 9: Properties of each reactant.

Id	Name	SBO
M	M	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \mathrm{vol}\,(\mathrm{system}) \cdot \mathrm{kmd} \cdot [\mathrm{M}] \tag{17}$$

8.4 Reaction r4

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

Name r4

Reaction equation

$$\emptyset \xrightarrow{\mathrm{M}} \mathrm{CP} \tag{18}$$

Modifier

Table 10: Properties of each modifier.

Id	Name	SBO
M	M	

Product

Table 11: Properties of each product.

Id	Name	SBO
CP	CP	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \mathrm{vol}\,(\mathrm{system}) \cdot \mathrm{function\_1}\,(\mathrm{kcps}, [\mathrm{M}]) \tag{19}$$

$$\mathrm{function\_1}\,(\mathrm{kcps}, [\mathrm{M}]) = \mathrm{kcps} \cdot [\mathrm{M}] \tag{20}$$

$$\mathrm{function\_1}\,(\mathrm{kcps}, [\mathrm{M}]) = \mathrm{kcps} \cdot [\mathrm{M}] \tag{21}$$

8.5 Reaction r5

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

Name r5

Reaction equation

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

Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
CP	CP	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \mathrm{vol}\,(\mathrm{system}) \cdot \mathrm{kcpd} \cdot [\mathrm{CP}] \tag{23}$$

8.6 Reaction r6

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

Name r6

Reaction equation

$$2\,\mathrm{CP} \longrightarrow \mathrm{CP2} \tag{24}$$

Reactant

Table 13: Properties of each reactant.

Id	Name	SBO
CP	CP	

Product

Table 14: Properties of each product.

Id	Name	SBO
CP2	CP2	

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \mathrm{vol}\,(\mathrm{system}) \cdot \mathrm{ka} \cdot [\mathrm{CP}]^2 \tag{25}$$

8.7 Reaction r7

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

Name r7

Reaction equation

$$\mathrm{CP2} \longrightarrow 2\,\mathrm{CP} \tag{26}$$

Reactant

Table 15: Properties of each reactant.

Id	Name	SBO
CP2	CP2	

Product

Table 16: Properties of each product.

Id	Name	SBO
CP	CP	

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \mathrm{vol}\,(\mathrm{system}) \cdot \mathrm{kd} \cdot [\mathrm{CP2}] \tag{27}$$

8.8 Reaction r8

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

Name r8

Reaction equation

$$\mathrm{CP} \xrightarrow{\mathrm{CP2,\ IC}} \emptyset \tag{28}$$

Reactant

Table 17: Properties of each reactant.

Id	Name	SBO
CP	CP	

Modifiers

Table 18: Properties of each modifier.

Id	Name	SBO
CP2	CP2	
IC	IC	

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \mathrm{vol}\left(\mathrm{system}\right) \cdot \mathrm{function\_4\_r8}\left(\left[\mathrm{CP}\right], \left[\mathrm{CP2}\right], \left[\mathrm{IC}\right], \mathrm{Jp}, \mathrm{kp1}, \mathrm{vol}\left(\mathrm{system}\right)\right) \tag{29}$$

$$\mathrm{function\_4\_r8}\left(\left[\mathrm{CP}\right], \left[\mathrm{CP2}\right], \left[\mathrm{IC}\right], \mathrm{Jp}, \mathrm{kp1}, \mathrm{vol}\left(\mathrm{system}\right)\right) = \frac{\frac{\mathrm{kp1} \cdot \left[\mathrm{CP}\right]}{\mathrm{Jp} + \left[\mathrm{CP}\right] + 2 \cdot \left[\mathrm{CP2}\right] + 2 \cdot \left[\mathrm{IC}\right]}}{\mathrm{vol}\left(\mathrm{system}\right)} \tag{30}$$

$$\mathrm{function\_4\_r8}\left(\left[\mathrm{CP}\right], \left[\mathrm{CP2}\right], \left[\mathrm{IC}\right], \mathrm{Jp}, \mathrm{kp1}, \mathrm{vol}\left(\mathrm{system}\right)\right) = \frac{\frac{\mathrm{kp1} \cdot \left[\mathrm{CP}\right]}{\mathrm{Jp} + \left[\mathrm{CP}\right] + 2 \cdot \left[\mathrm{CP2}\right] + 2 \cdot \left[\mathrm{IC}\right]}}{\mathrm{vol}\left(\mathrm{system}\right)} \tag{31}$$

8.9 Reaction r9

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

Name r9

Reaction equation

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

Reactant

Table 19: Properties of each reactant.

Id	Name	SBO
CP	CP	

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \mathrm{vol}\,(\mathrm{system}) \cdot \mathrm{chk2} \cdot [\mathrm{CP}] \tag{33}$$

8.10 Reaction r10

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

Name r10

Reaction equation

$$\mathrm{IC} \longrightarrow \mathrm{CP2} + \mathrm{TF} \tag{34}$$

Reactant

Table 20: Properties of each reactant.

Id	Name	SBO
IC	IC	

Products

Table 21: Properties of each product.

Id	Name	SBO
CP2	CP2	
TF	TF	

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = \mathrm{vol}\,(\mathrm{system}) \cdot \mathrm{kicd} \cdot [\mathrm{IC}] \tag{35}$$

8.11 Reaction r11

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

Name r11

Reaction equation

$$\mathrm{CP2} \longrightarrow \emptyset \tag{36}$$

Reactant

Table 22: Properties of each reactant.

Id	Name	SBO
CP2	CP2	

Kinetic Law

Derived unit contains undeclared units

$$v_{11} = \mathrm{vol}(\mathrm{system}) \cdot \mathrm{kcp2d} \cdot [\mathrm{CP2}] \tag{37}$$

8.12 Reaction r12

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

Name r12

Reaction equation

$$\mathrm{CP2} + \mathrm{TF} \longrightarrow \mathrm{IC} \tag{38}$$

Reactants

Table 23: Properties of each reactant.

Id	Name	SBO
CP2	CP2	
TF	TF	

Product

Table 24: Properties of each product.

Id	Name	SBO
IC	IC	

Kinetic Law

Derived unit contains undeclared units

$$v_{12} = \mathrm{vol}\,(\mathrm{system}) \cdot \mathrm{kica} \cdot [\mathrm{CP2}] \cdot [\mathrm{TF}] \tag{39}$$

8.13 Reaction r13

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

Name r13

Reaction equation

$$\mathrm{CP2} \xrightarrow{\mathrm{CP,\ IC}} \emptyset \tag{40}$$

Reactant

Table 25: Properties of each reactant.

Id	Name	SBO
CP2	CP2	

Modifiers

Table 26: Properties of each modifier.

Id	Name	SBO
CP	CP	
IC	IC	

Kinetic Law

Derived unit contains undeclared units

$$v_{13} = \mathrm{vol}\,(\mathrm{system}) \cdot \mathrm{function\_4\_r13}\,([\mathrm{CP}], [\mathrm{CP2}], [\mathrm{IC}], \mathrm{Jp}, \mathrm{kp2}, \mathrm{vol}\,(\mathrm{system})) \tag{41}$$

$$\text{function\_4\_r13}\left([\text{CP}],[\text{CP2}],[\text{IC}],\text{Jp},\text{kp2},\text{vol}\left(\text{system}\right)\right) = \frac{\frac{\text{kp2}\cdot[\text{CP2}]}{\text{Jp}+[\text{CP}]+2\cdot[\text{CP2}]+2\cdot[\text{IC}]}}{\text{vol}\left(\text{system}\right)} \tag{42}$$

$$\text{function\_4\_r13}\left([\text{CP}],[\text{CP2}],[\text{IC}],\text{Jp},\text{kp2},\text{vol}\left(\text{system}\right)\right) = \frac{\frac{\text{kp2}\cdot[\text{CP2}]}{\text{Jp}+[\text{CP}]+2\cdot[\text{CP2}]+2\cdot[\text{IC}]}}{\text{vol}\left(\text{system}\right)} \tag{43}$$

8.14 Reaction `r14`

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

Name r14

Reaction equation

$$\text{CP2} \longrightarrow \emptyset \tag{44}$$

Reactant

Table 27: Properties of each reactant.

Id	Name	SBO
`CP2`	CP2	

Kinetic Law

Derived unit contains undeclared units

$$v_{14} = \text{vol}\left(\text{system}\right) \cdot \text{chk2} \cdot [\text{CP2}] \tag{45}$$

8.15 Reaction `r15`

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

Name r15

Reaction equation

$$\text{IC} \longrightarrow \text{TF} \tag{46}$$

Reactant

Table 28: Properties of each reactant.

Id	Name	SBO
IC	IC	

Product

Table 29: Properties of each product.

Id	Name	SBO
TF	TF	

Kinetic Law

Derived unit contains undeclared units

$$v_{15} = \mathrm{vol}\,(\mathrm{system}) \cdot \mathrm{kcp2d} \cdot [\mathrm{IC}] \tag{47}$$

8.16 Reaction r16

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

Name r16

Reaction equation

$$\mathrm{IC} \longrightarrow \mathrm{TF} \tag{48}$$

Reactant

Table 30: Properties of each reactant.

Id	Name	SBO
IC	IC	

Product

Table 31: Properties of each product.

Id	Name	SBO
TF	TF	

Kinetic Law

Derived unit contains undeclared units

$$v_{16} = \mathrm{vol}\,(\mathrm{system}) \cdot \mathrm{chk2c} \cdot [\mathrm{IC}] \tag{49}$$

8.17 Reaction r17

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

Name r17

Reaction equation

$$\mathrm{IC} \xrightarrow{\mathrm{CP2,\ CP}} \mathrm{TF} \tag{50}$$

Reactant

Table 32: Properties of each reactant.

Id	Name	SBO
IC	IC	

Modifiers

Table 33: Properties of each modifier.

Id	Name	SBO
CP2	CP2	
CP	CP	

Product

Table 34: Properties of each product.

Id	Name	SBO
TF	TF	

Kinetic Law

Derived unit contains undeclared units

$$v_{17} = \mathrm{vol}\,(\mathrm{system}) \cdot \mathrm{function\_4\_r17}\,([\mathrm{CP}], [\mathrm{CP2}], [\mathrm{IC}], \mathrm{Jp}, \mathrm{kp2}, \mathrm{vol}\,(\mathrm{system})) \tag{51}$$

$$\mathrm{function\_4\_r17}\,([\mathrm{CP}], [\mathrm{CP2}], [\mathrm{IC}], \mathrm{Jp}, \mathrm{kp2}, \mathrm{vol}\,(\mathrm{system})) = \frac{\frac{\mathrm{kp2} \cdot [\mathrm{IC}]}{\mathrm{Jp} + [\mathrm{CP}] + 2 \cdot [\mathrm{CP2}] + 2 \cdot [\mathrm{IC}]}}{\mathrm{vol}\,(\mathrm{system})} \tag{52}$$

$$\mathrm{function\_4\_r17}\,([\mathrm{CP}], [\mathrm{CP2}], [\mathrm{IC}], \mathrm{Jp}, \mathrm{kp2}, \mathrm{vol}\,(\mathrm{system})) = \frac{\frac{\mathrm{kp2} \cdot [\mathrm{IC}]}{\mathrm{Jp} + [\mathrm{CP}] + 2 \cdot [\mathrm{CP2}] + 2 \cdot [\mathrm{IC}]}}{\mathrm{vol}\,(\mathrm{system})} \tag{53}$$

9 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.

9.1 Species `M`

Name M

SBO:0000278 messenger RNA

Initial concentration $1.4\ \mathrm{mol} \cdot \mathrm{l}^{-1}$

This species takes part in four reactions (as a reactant in `r3` and as a product in `r1`, `r2` and as a modifier in `r4`).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{M} = v_1 + v_2 - v_3 \tag{54}$$

9.2 Species `TF`

Name TF

SBO:0000296 macromolecular complex

Initial concentration $0.13\ \mathrm{mol} \cdot \mathrm{l}^{-1}$

This species takes part in six reactions (as a reactant in `r12` and as a product in `r10`, `r15`, `r16`, `r17` and as a modifier in `r2`).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{TF} = v_{10} + v_{15} + v_{16} + v_{17} - v_{12} \tag{55}$$

9.3 Species CP

Name CP

SBO:0000252 polypeptide chain

Initial concentration $0.037\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in eight reactions (as a reactant in r5, r6, r8, r9 and as a product in r4, r7 and as a modifier in r13, r17).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{CP} = v_4 + 2\,v_7 - v_5 - 2\,v_6 - v_8 - v_9 \tag{56}$$

9.4 Species CP2

Name CP2

SBO:0000297 protein complex

Initial concentration $0.046\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in nine reactions (as a reactant in r7, r11, r12, r13, r14 and as a product in r6, r10 and as a modifier in r8, r17).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{CP2} = v_6 + v_{10} - v_7 - v_{11} - v_{12} - v_{13} - v_{14} \tag{57}$$

9.5 Species IC

Name IC

SBO:0000296 macromolecular complex

Notes Inactive complex of clock dimers and transcription factor: IC= TFtot-TF

Initial concentration $0.37\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in seven reactions (as a reactant in r10, r15, r16, r17 and as a product in r12 and as a modifier in r8, r13).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{IC} = v_{12} - v_{10} - v_{15} - v_{16} - v_{17} \tag{58}$$

9.6 Species CPtot

Name CPtot

Involved in rule CPtot

One rule determines the species' quantity.

A Glossary of Systems Biology Ontology Terms

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

SBO:0000252 polypeptide chain: Naturally occurring macromolecule formed by the repetition of amino-acid residues linked by peptidic bonds. A polypeptide chain is synthesized by the ribosome. CHEBI:1654

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:0000296 macromolecular complex: Non-covalent complex of one or more macromolecules and zero or more simple chemicals

SBO:0000297 protein complex: Macromolecular complex containing one or more polypeptide chains possibly associated with simple chemicals. CHEBI:3608

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.

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