

SBML Model Report

Model name: “Locke2008_Circadian_Clock”



May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 3 format. This model was created by Harish Dharuri¹ at August 20th 2008 at 8:10 a.m. and last time modified at July eleventh 2012 at 5:47 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	8
events	0	constraints	0
reactions	20	function definitions	0
global parameters	19	unit definitions	5
rules	1	initial assignments	0

Model Notes

The model reproduces Fig 2A of the paper. Model successfully reproduced using Jarnac and MathSBML.

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2 Unit Definitions

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

2.1 Unit `substance`

Name nano mole

Definition nmol

2.2 Unit `time`

Name hour

Definition 3600 s

2.3 Unit `nM`

Name nM

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

2.4 Unit `nM_hr_1`

Name nM_hr_1

Definition $\text{nmol} \cdot \text{l}^{-1} \cdot (3600 \text{ s})^{-1}$

2.5 Unit `hr_1`

Name hr_1

Definition $(3600 \text{ s})^{-1}$

2.6 Unit `volume`

Notes Litre is the predefined SBML unit for volume.

Definition l

2.7 Unit `area`

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

Definition m^2

2.8 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
<code>compartment</code>	Cell		3	1	litre	<input checked="" type="checkbox"/>	

3.1 Compartment `compartment`

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

Name Cell

4 Species

This model contains eight species. 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
X1	clock gene mRNA	compartment	$\text{nmol} \cdot \text{l}^{-1}$	\square	\square
Y1	clock protein	compartment	$\text{nmol} \cdot \text{l}^{-1}$	\square	\square
Z1	Transcriptional repressor	compartment	$\text{nmol} \cdot \text{l}^{-1}$	\square	\square
V1	Neuropeptide	compartment	$\text{nmol} \cdot \text{l}^{-1}$	\square	\square
X2	clock gene mRNA	compartment	$\text{nmol} \cdot \text{l}^{-1}$	\square	\square
Y2	clock protein	compartment	$\text{nmol} \cdot \text{l}^{-1}$	\square	\square
Z2	Transcriptional repressor	compartment	$\text{nmol} \cdot \text{l}^{-1}$	\square	\square
V2	Neuropeptide	compartment	$\text{nmol} \cdot \text{l}^{-1}$	\square	\square

5 Parameters

This model contains 19 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
F			0.000	$\text{nmol} \cdot \text{l}^{-1}$	<input type="checkbox"/>
v_1			6.836	$\text{nmol} \cdot \text{l}^{-1} \cdot (3600 \text{ s})^{-1}$	<input checked="" type="checkbox"/>
K1			2.727	$\text{nmol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>
n			5.665	dimensionless	<input checked="" type="checkbox"/>
v_2			8.430	$\text{nmol} \cdot \text{l}^{-1} \cdot (3600 \text{ s})^{-1}$	<input checked="" type="checkbox"/>
K2			0.291	$\text{nmol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>
vc			6.792	$\text{nmol} \cdot \text{l}^{-1} \cdot (3600 \text{ s})^{-1}$	<input checked="" type="checkbox"/>
K			1.000	dimensionless	<input checked="" type="checkbox"/>
Kc			4.828	$\text{nmol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>
L			0.000	$\text{nmol} \cdot \text{l}^{-1} \cdot (3600 \text{ s})^{-1}$	<input checked="" type="checkbox"/>
k3			0.118	$(3600 \text{ s})^{-1}$	<input checked="" type="checkbox"/>
v_4			1.084	$\text{nmol} \cdot \text{l}^{-1} \cdot (3600 \text{ s})^{-1}$	<input checked="" type="checkbox"/>
K4			8.134	$\text{nmol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>
k5			0.335	$(3600 \text{ s})^{-1}$	<input checked="" type="checkbox"/>
v_6			4.665	$\text{nmol} \cdot \text{l}^{-1} \cdot (3600 \text{ s})^{-1}$	<input checked="" type="checkbox"/>
K6			9.985	$\text{nmol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>
k7			0.228	$(3600 \text{ s})^{-1}$	<input checked="" type="checkbox"/>
v_8			3.522	$\text{nmol} \cdot \text{l}^{-1} \cdot (3600 \text{ s})^{-1}$	<input checked="" type="checkbox"/>
K8			7.452	$\text{nmol} \cdot \text{l}^{-1}$	<input checked="" type="checkbox"/>

6 Rule

This is an overview of one rule.

6.1 Rule F

Rule F is an assignment rule for parameter F:

$$F = \frac{1}{2} \cdot ([V1] + [V2]) \quad (1)$$

7 Reactions

This model contains 20 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	R1	Transcription	$\emptyset \xrightarrow{Z1} X1$	
2	R2	mRNA degradation	$X1 \longrightarrow \emptyset$	
3	R3	Neuropeptide dependent transcription activation	$\emptyset \longrightarrow X1$	
4	R4	Light dependent transcription activation	$\emptyset \longrightarrow X1$	
5	R5	Translation	$\emptyset \xrightarrow{X1} Y1$	
6	R6	Protein degradation	$Y1 \longrightarrow \emptyset$	
7	R7	Transcriptional repressor synthesis	$\emptyset \xrightarrow{Y1} Z1$	
8	R8	Transcriptional repressor degradation	$Z1 \longrightarrow \emptyset$	
9	R9	Neuropeptide synthesis	$\emptyset \xrightarrow{X1} V1$	
10	R10	Neuropeptide degradation	$V1 \longrightarrow \emptyset$	
11	R11	Transcription	$\emptyset \xrightarrow{Z2} X2$	
12	R12	mRNA degradation	$X2 \longrightarrow \emptyset$	
13	R13	Neuropeptide dependent transcription activation	$\emptyset \longrightarrow X2$	
14	R14	Light dependent transcription activation	$\emptyset \longrightarrow X2$	
15	R15	Translation	$\emptyset \xrightarrow{X2} Y2$	
16	R16	Protein degradation	$Y2 \longrightarrow \emptyset$	
17	R17	Transcriptional repressor synthesis	$\emptyset \xrightarrow{Y2} Z2$	
18	R18	Transcriptional repressor degradation	$Z2 \longrightarrow \emptyset$	

Nº	Id	Name	Reaction Equation	SBO
19	R19	Neuropeptide synthesis	$\emptyset \xrightarrow{X2} V2$	
20	R20	Neuropeptide degradation	$V2 \longrightarrow \emptyset$	

7.1 Reaction R1

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

Name Transcription

Reaction equation



Modifier

Table 6: Properties of each modifier.

Id	Name	SBO
Z1	Transcriptional repressor	

Product

Table 7: Properties of each product.

Id	Name	SBO
X1	clock gene mRNA	

Kinetic Law

Derived unit contains undeclared units

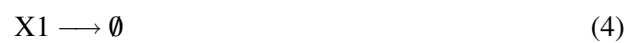
$$v_1 = \frac{\text{vol}(\text{compartment}) \cdot v_{-1} \cdot K1^n}{K1^n + [Z1]^n} \quad (3)$$

7.2 Reaction R2

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

Name mRNA degradation

Reaction equation



Reactant

Table 8: Properties of each reactant.

Id	Name	SBO
X1	clock gene mRNA	

Kinetic Law

Derived unit $9.99999999999998 \cdot 10^{-10} \text{ mol} \cdot (3600 \text{ s})^{-1}$

$$v_2 = \frac{\text{vol}(\text{compartment}) \cdot v_2 \cdot [\text{X1}]}{K_2 + [\text{X1}]} \quad (5)$$

7.3 Reaction R3

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

Name Neuropeptide dependent transcription activation

Reaction equation



Product

Table 9: Properties of each product.

Id	Name	SBO
X1	clock gene mRNA	

Kinetic Law

Derived unit $9.99999999999998 \cdot 10^{-10} \text{ mol} \cdot (3600 \text{ s})^{-1}$

$$v_3 = \frac{\text{vol}(\text{compartment}) \cdot v_c \cdot K \cdot F}{K_c + K \cdot F} \quad (7)$$

7.4 Reaction R4

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

Name Light dependent transcription activation

Reaction equation



Product

Table 10: Properties of each product.

Id	Name	SBO
X1	clock gene mRNA	

Kinetic Law

Derived unit $\text{nmol} \cdot (3600 \text{ s})^{-1}$

$$v_4 = \text{vol}(\text{compartment}) \cdot L \quad (9)$$

7.5 Reaction R5

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

Name Translation

Reaction equation



Modifier

Table 11: Properties of each modifier.

Id	Name	SBO
X1	clock gene mRNA	

Product

Table 12: Properties of each product.

Id	Name	SBO
Y1	clock protein	

Kinetic Law

Derived unit $(3600 \text{ s})^{-1} \cdot \text{nmol}$

$$v_5 = \text{vol}(\text{compartment}) \cdot k3 \cdot [X1] \quad (11)$$

7.6 Reaction R6

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

Name Protein degradation

Reaction equation



Reactant

Table 13: Properties of each reactant.

Id	Name	SBO
Y1	clock protein	

Kinetic Law

Derived unit $9.999999999999998 \cdot 10^{-10} \text{ mol} \cdot (3600 \text{ s})^{-1}$

$$v_6 = \frac{\text{vol}(\text{compartment}) \cdot v_4 \cdot [Y1]}{K4 + [Y1]} \quad (13)$$

7.7 Reaction R7

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

Name Transcriptional repressor synthesis

Reaction equation



Modifier

Table 14: Properties of each modifier.

Id	Name	SBO
Y1	clock protein	

Product

Table 15: Properties of each product.

Id	Name	SBO
Z1	Transcriptional repressor	

Kinetic Law

Derived unit $(3600 \text{ s})^{-1} \cdot \text{nmol}$

$$v_7 = \text{vol}(\text{compartment}) \cdot k_5 \cdot [Y1] \quad (15)$$

7.8 Reaction R8

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

Name Transcriptional repressor degradation

Reaction equation



Reactant

Table 16: Properties of each reactant.

Id	Name	SBO
Z1	Transcriptional repressor	

Kinetic Law

Derived unit $9.999999999999998 \cdot 10^{-10} \text{ mol} \cdot (3600 \text{ s})^{-1}$

$$v_8 = \frac{\text{vol}(\text{compartment}) \cdot v_6 \cdot [Z1]}{K6 + [Z1]} \quad (17)$$

7.9 Reaction R9

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

Name Neuropeptide synthesis

Reaction equation



Modifier

Table 17: Properties of each modifier.

Id	Name	SBO
X1	clock gene mRNA	

Product

Table 18: Properties of each product.

Id	Name	SBO
V1	Neuropeptide	

Kinetic Law

Derived unit $(3600\text{ s})^{-1} \cdot \text{nmol}$

$$v_9 = \text{vol}(\text{compartment}) \cdot k_7 \cdot [\text{X1}] \quad (19)$$

7.10 Reaction R10

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

Name Neuropeptide degradation

Reaction equation



Reactant

Table 19: Properties of each reactant.

Id	Name	SBO
V1	Neuropeptide	

Kinetic Law

Derived unit $9.999999999999998 \cdot 10^{-10} \text{ mol} \cdot (3600\text{ s})^{-1}$

$$v_{10} = \frac{\text{vol}(\text{compartment}) \cdot v_{-8} \cdot [V1]}{K8 + [V1]} \quad (21)$$

7.11 Reaction R11

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

Name Transcription

Reaction equation



Modifier

Table 20: Properties of each modifier.

Id	Name	SBO
Z2	Transcriptional repressor	

Product

Table 21: Properties of each product.

Id	Name	SBO
X2	clock gene mRNA	

Kinetic Law

Derived unit contains undeclared units

$$v_{11} = \frac{\text{vol}(\text{compartment}) \cdot v_{-1} \cdot K1^n}{K1^n + [Z2]^n} \quad (23)$$

7.12 Reaction R12

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

Name mRNA degradation

Reaction equation



Reactant

Table 22: Properties of each reactant.

Id	Name	SBO
X2	clock gene mRNA	

Kinetic Law

Derived unit $9.999999999999998 \cdot 10^{-10} \text{ mol} \cdot (3600 \text{ s})^{-1}$

$$v_{12} = \frac{\text{vol}(\text{compartment}) \cdot v_2 \cdot [\text{X2}]}{K_2 + [\text{X2}]} \quad (25)$$

7.13 Reaction R13

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

Name Neuropeptide dependent transcription activation

Reaction equation



Product

Table 23: Properties of each product.

Id	Name	SBO
X2	clock gene mRNA	

Kinetic Law

Derived unit $9.999999999999998 \cdot 10^{-10} \text{ mol} \cdot (3600 \text{ s})^{-1}$

$$v_{13} = \frac{\text{vol}(\text{compartment}) \cdot v_c \cdot K \cdot F}{K_c + K \cdot F} \quad (27)$$

7.14 Reaction R14

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

Name Light dependent transcription activation

Reaction equation



Product

Table 24: Properties of each product.

Id	Name	SBO
X2	clock gene mRNA	

Kinetic Law

Derived unit $\text{nmol} \cdot (3600 \text{ s})^{-1}$

$$v_{14} = \text{vol}(\text{compartment}) \cdot L \quad (29)$$

7.15 Reaction R15

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

Name Translation

Reaction equation



Modifier

Table 25: Properties of each modifier.

Id	Name	SBO
X2	clock gene mRNA	

Product

Table 26: Properties of each product.

Id	Name	SBO
Y2	clock protein	

Kinetic Law

Derived unit $(3600\text{ s})^{-1} \cdot \text{nmol}$

$$v_{15} = \text{vol}(\text{compartment}) \cdot k_3 \cdot [\text{X2}] \quad (31)$$

7.16 Reaction R16

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

Name Protein degradation

Reaction equation



Reactant

Table 27: Properties of each reactant.

Id	Name	SBO
Y2	clock protein	

Kinetic Law

Derived unit $9.999999999999998 \cdot 10^{-10} \text{ mol} \cdot (3600\text{ s})^{-1}$

$$v_{16} = \frac{\text{vol}(\text{compartment}) \cdot v_4 \cdot [\text{Y2}]}{K_4 + [\text{Y2}]} \quad (33)$$

7.17 Reaction R17

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

Name Transcriptional repressor synthesis

Reaction equation



Modifier

Table 28: Properties of each modifier.

Id	Name	SBO
Y2	clock protein	

Product

Table 29: Properties of each product.

Id	Name	SBO
Z2	Transcriptional repressor	

Kinetic Law

Derived unit $(3600 \text{ s})^{-1} \cdot \text{nmol}$

$$v_{17} = \text{vol}(\text{compartment}) \cdot k5 \cdot [\text{Y2}] \quad (35)$$

7.18 Reaction R18

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

Name Transcriptional repressor degradation

Reaction equation



Reactant

Table 30: Properties of each reactant.

Id	Name	SBO
Z2	Transcriptional repressor	

Kinetic Law

Derived unit $9.999999999999998 \cdot 10^{-10} \text{ mol} \cdot (3600 \text{ s})^{-1}$

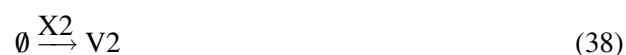
$$v_{18} = \frac{\text{vol}(\text{compartment}) \cdot v_6 \cdot [\text{Z2}]}{K6 + [\text{Z2}]} \quad (37)$$

7.19 Reaction R19

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

Name Neuropeptide synthesis

Reaction equation



Modifier

Table 31: Properties of each modifier.

Id	Name	SBO
X2	clock gene mRNA	

Product

Table 32: Properties of each product.

Id	Name	SBO
V2	Neuropeptide	

Kinetic Law

Derived unit $(3600 \text{ s})^{-1} \cdot \text{nmol}$

$$v_{19} = \text{vol}(\text{compartment}) \cdot k7 \cdot [X2] \quad (39)$$

7.20 Reaction R20

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

Name Neuropeptide degradation

Reaction equation



Reactant

Table 33: Properties of each reactant.

Id	Name	SBO
V2	Neuropeptide	

Kinetic Law

Derived unit $9.999999999999998 \cdot 10^{-10} \text{ mol} \cdot (3600 \text{ s})^{-1}$

$$v_{20} = \frac{\text{vol}(\text{compartment}) \cdot v_{\text{8}} \cdot [\text{V2}]}{K8 + [\text{V2}]} \quad (41)$$

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 X1

Name clock gene mRNA

Initial concentration $4.25 \text{ nmol} \cdot \text{l}^{-1}$

This species takes part in six reactions (as a reactant in [R2](#) and as a product in [R1](#), [R3](#), [R4](#) and as a modifier in [R5](#), [R9](#)).

$$\frac{d}{dt}X1 = v_1 + v_3 + v_4 - v_2 \quad (42)$$

8.2 Species Y1

Name clock protein

Initial concentration $3.25 \text{ nmol} \cdot \text{l}^{-1}$

This species takes part in three reactions (as a reactant in [R6](#) and as a product in [R5](#) and as a modifier in [R7](#)).

$$\frac{d}{dt}Y1 = v_5 - v_6 \quad (43)$$

8.3 Species Z1

Name Transcriptional repressor

Initial concentration $2.25 \text{ nmol} \cdot \text{l}^{-1}$

This species takes part in three reactions (as a reactant in R8 and as a product in R7 and as a modifier in R1).

$$\frac{d}{dt}Z1 = v_7 - v_8 \quad (44)$$

8.4 Species V1

Name Neuropeptide

Initial concentration $2.5 \text{ nmol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a reactant in R10 and as a product in R9).

$$\frac{d}{dt}V1 = v_9 - v_{10} \quad (45)$$

8.5 Species X2

Name clock gene mRNA

Initial concentration $0 \text{ nmol} \cdot \text{l}^{-1}$

This species takes part in six reactions (as a reactant in R12 and as a product in R11, R13, R14 and as a modifier in R15, R19).

$$\frac{d}{dt}X2 = v_{11} + v_{13} + v_{14} - v_{12} \quad (46)$$

8.6 Species Y2

Name clock protein

Initial concentration $0 \text{ nmol} \cdot \text{l}^{-1}$

This species takes part in three reactions (as a reactant in R16 and as a product in R15 and as a modifier in R17).

$$\frac{d}{dt}Y2 = v_{15} - v_{16} \quad (47)$$

8.7 Species Z2

Name Transcriptional repressor

Initial concentration 0 nmol · l⁻¹

This species takes part in three reactions (as a reactant in R18 and as a product in R17 and as a modifier in R11).

$$\frac{d}{dt}Z2 = v_{17} - v_{18} \quad (48)$$

8.8 Species V2

Name Neuropeptide

Initial concentration 0 nmol · l⁻¹

This species takes part in two reactions (as a reactant in R20 and as a product in R19).

$$\frac{d}{dt}V2 = v_{19} - v_{20} \quad (49)$$

SBML2^{AT}EX 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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