SBML Model Report

Model name: "Heiland2012_CircadianClock_C.reinhardtii"

May 5, 2016

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by the following two authors: Vijayalakshmi Chelliah[1] and Ines Heiland[2] at April second 2012 at 3:49 p. m. and last time modified at February fifth 2014 at 12:45 a. 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	13	function definitions	5
global parameters	12	unit definitions	2
rules	3	initial assignments	0

Model Notes

This model is from the article:
Modeling temperature entrainment of circadian clocks using the Arrhenius equation and a reconstructed model from Chlamydomonas reinhardtii

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Ines Heiland, Christian Bodenstein, Thomas Hinze, Olga Weisheit, Oliver Ebenhoeh, Maria Mittag and Stefan Schuster Journal of Biological Physics 4 March 2012; pp 1-16; doi: 10.1007/s10867-012-9264-x ,

Abstract:
Endogenous circadian rhythms allow living organisms to anticipate daily variations in their natural environment. Temperature regulation and entrainment mechanisms of circadian clocks are still poorly understood. To better understand the molecular basis of these processes, we built a mathematical model based on experimental data examining temperature regulation of the circadian RNA-binding protein CHLAMY1 from the unicellular green alga Chlamydomonas reinhardtii , simulating the effect of temperature on the rates by applying the Arrhenius equation. Using numerical simulations, we demonstrate that our model is temperature-compensated and can be entrained to temperature cycles of various length and amplitude. The range of periods that allow entrainment of the model depends on the shape of the temperature cycles and is larger for sinusoidal compared to rectangular temperature curves. We show that the response to temperature of protein (de)phosphorylation rates play a key role in facilitating temperature entrainment of the oscillator in Chlamydomonas reinhardtii . We systematically investigated the response of our model to single temperature pulses to explain experimentally observed phase response curves.

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 `time`

Name time

Definition 3600 s

2.2 Unit `substance`

Name substance

Definition nmol

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 2: Properties of all compartments.

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

3.1 Compartment default

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

Name default

SBO:0000290 physical compartment

4 Species

This model contains ten species. The boundary condition of three of these species is set to `true` so that these 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
`s2`	C3_Gene	`default`	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	☑	☑
`s9`	C3_mRNA	`default`	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	☐	☐
`s10`	C_3	`default`	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	☐	☐
`s11`	C_3_P	`default`	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	☐	☐
`s13`	C_3_pre	`default`	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	☑	☑
`species_1`	C1	`default`	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	☐	☐
`species_2`	C1_mRNA	`default`	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	☑	☑
`species_3`	C1_phos	`default`	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	☐	☐
`species_4`	c1c3complex	`default`	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	☐	☐
`species_12`	junk	`default`	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	☐	☐

5 Parameters

This model contains twelve global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
T	T	0000147	291.000		☑
T2	T2		296.000		⊟
parameter_1	v_phos		1.000		☑
parameter_2	V_dephos		0.500		☑
parameter_3	R		8.314		☑
parameter_4	amplitude		10.000		☑
parameter_5	entrperiod		24.000		☑
parameter_6	EAlow		50000.000		⊟
parameter_7	EAhigh		84000.000		⊟
parameter_8	vphosdegr		1.000		☑
parameter_9	Ephos		60000.000		☑
parameter_10	Edephos		67000.000		☑

6 Function definitions

This is an overview of five function definitions.

6.1 Function definition function_2

Name arhenius neg feedb tempvar

Arguments v, E, R, T2, T1, k, S, h

Mathematical Expression

$$\frac{\mathrm{v} \cdot \exp\left(\frac{\frac{\mathrm{E}}{\mathrm{R}} \cdot (\mathrm{T2} - \mathrm{T1})}{\mathrm{T1} \cdot \mathrm{T2}}\right)}{\mathrm{k} + \mathrm{S}^{\mathrm{h}}} \tag{1}$$

6.2 Function definition function_1

Name arhenius mass action tempvar

Arguments v, E, R, T2, T1, S

Mathematical Expression

$$\mathrm{v} \cdot \exp\left(\frac{\frac{\mathrm{E}}{\mathrm{R}} \cdot (\mathrm{T2} - \mathrm{T1})}{\mathrm{T1} \cdot \mathrm{T2}}\right) \cdot \mathrm{S} \tag{2}$$

6.3 Function definition function_4

Name arhenius tranls temp var

Arguments v, E, R, T2, T1, S

Mathematical Expression

$$\mathrm{v} \cdot \exp\left(\frac{\frac{\mathrm{E}}{\mathrm{R}} \cdot (\mathrm{T2} - \mathrm{T1})}{\mathrm{T1} \cdot \mathrm{T2}}\right) \cdot \mathrm{S} \tag{3}$$

6.4 Function definition function_3

Name arhenius michaelis menten temp var

Arguments v, E, R, T2, T1, S, Km

Mathematical Expression

$$\frac{\mathrm{v} \cdot \exp\left(\frac{\frac{\mathrm{E}}{\mathrm{R}} \cdot (\mathrm{T2} - \mathrm{T1})}{\mathrm{T1} \cdot \mathrm{T2}}\right) \cdot \mathrm{S}}{\mathrm{Km} + \mathrm{S}} \tag{4}$$

6.5 Function definition function_5

Name arhenius complexf temp var

Arguments v, E, R, T2, T1, S1, S2, a

Mathematical Expression

$$\mathrm{v} \cdot \exp\left(\frac{\frac{\mathrm{E}}{\mathrm{R}} \cdot (\mathrm{T2} - \mathrm{T1})}{\mathrm{T1} \cdot \mathrm{T2}}\right) \cdot \mathrm{S1} \cdot \mathrm{S2}^{\mathrm{a}} \tag{5}$$

7 Rules

This is an overview of three rules.

7.1 Rule T2

Rule T2 is an assignment rule for parameter T2:

$$\mathrm{T2} = 296 + \frac{\mathrm{parameter\_4}}{2} \cdot \sin\left(\frac{2 \cdot \pi \cdot \mathrm{time}}{\mathrm{parameter\_5}}\right) \tag{6}$$

7.2 Rule parameter_6

Rule parameter_6 is an assignment rule for parameter parameter_6:

$$\mathrm{parameter\_6} = 50000 \tag{7}$$

7.3 Rule parameter_7

Rule parameter_7 is an assignment rule for parameter parameter_7:

$$\text{parameter\_7} = 84000 \tag{8}$$

8 Reactions

This model contains 13 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	re12	C3_phos	s10 $\longrightarrow$ s11	0000216
2	re13	C3_transk	s2 $\xrightarrow{\text{s11}}$ s9	0000183
3	re14	C3_mRNADegr	s9 $\longrightarrow$ species_12	0000179
4	re15	C3_degr	s10 $\longrightarrow$ species_12	0000179
5	re16	C3_phos_degr	s11 $\longrightarrow$ species_12	0000179
6	re18	C3_transl	s13 $\xrightarrow{\text{s9}}$ s10	0000184
7	reaction_1	C1_transl	species_2 $\longrightarrow$ species_1	0000184
8	reaction_2	complexformation	species_3 + s11 $\longrightarrow$ species_4	0000526
9	reaction_3	C1_phos	species_1 $\longrightarrow$ species_3	0000216
10	reaction_4	C1_degr	species_1 $\longrightarrow$ species_12	0000179
11	reaction_5	complexdegr	species_4 $\longrightarrow$ species_12	0000179
12	reaction_6	C1_dephos	species_3 $\longrightarrow$ species_1	0000330
13	reaction_7	C1_phos_degr	species_3 $\longrightarrow$ species_12	0000179

8.1 Reaction re12

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

Name C3_phos

SBO:0000216 phosphorylation

Reaction equation

$$\mathrm{s10} \longrightarrow \mathrm{s11} \tag{9}$$

Reactant

Table 6: Properties of each reactant.

Id	Name	SBO
s10	C_3	

Product

Table 7: Properties of each product.

Id	Name	SBO
s11	C_3_P	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \mathrm{vol}\left(\mathrm{default}\right) \cdot \mathrm{function\_1}\left(\mathrm{v}, \mathrm{parameter\_6}, \mathrm{parameter\_3}, \mathrm{T2}, \mathrm{T}, [\mathrm{s10}]\right) \tag{10}$$

$$\mathrm{function\_1}\left(\mathrm{v}, \mathrm{E}, \mathrm{R}, \mathrm{T2}, \mathrm{T1}, \mathrm{S}\right) = \mathrm{v} \cdot \exp\left(\frac{\frac{\mathrm{E}}{\mathrm{R}} \cdot (\mathrm{T2} - \mathrm{T1})}{\mathrm{T1} \cdot \mathrm{T2}}\right) \cdot \mathrm{S} \tag{11}$$

$$\mathrm{function\_1}\left(\mathrm{v}, \mathrm{E}, \mathrm{R}, \mathrm{T2}, \mathrm{T1}, \mathrm{S}\right) = \mathrm{v} \cdot \exp\left(\frac{\frac{\mathrm{E}}{\mathrm{R}} \cdot (\mathrm{T2} - \mathrm{T1})}{\mathrm{T1} \cdot \mathrm{T2}}\right) \cdot \mathrm{S} \tag{12}$$

Table 8: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
v	v		0.1		☑

8.2 Reaction re13

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

Name C3_transk

SBO:0000183 transcription

Reaction equation

$$\mathrm{s2} \xrightarrow{\mathrm{s11}} \mathrm{s9} \tag{13}$$

Reactant

Table 9: Properties of each reactant.

Id	Name	SBO
s2	C3_Gene	

Modifier

Table 10: Properties of each modifier.

Id	Name	SBO
s11	C_3_P	

Product

Table 11: Properties of each product.

Id	Name	SBO
s9	C3_mRNA	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \mathrm{vol}\,(\mathrm{default}) \cdot \mathrm{function\_2}\,(\mathrm{v}, \mathrm{parameter\_7}, \mathrm{parameter\_3}, \mathrm{T2}, \mathrm{T}, \mathrm{k}, [\mathrm{s11}], \mathrm{h}) \tag{14}$$

$$\mathrm{function\_2}\,(\mathrm{v}, \mathrm{E}, \mathrm{R}, \mathrm{T2}, \mathrm{T1}, \mathrm{k}, \mathrm{S}, \mathrm{h}) = \frac{\mathrm{v} \cdot \exp\left(\frac{\frac{\mathrm{E}}{\mathrm{R}} \cdot (\mathrm{T2} - \mathrm{T1})}{\mathrm{T1} \cdot \mathrm{T2}}\right)}{\mathrm{k} + \mathrm{S}^{\mathrm{h}}} \tag{15}$$

$$\mathrm{function\_2}\,(\mathrm{v}, \mathrm{E}, \mathrm{R}, \mathrm{T2}, \mathrm{T1}, \mathrm{k}, \mathrm{S}, \mathrm{h}) = \frac{\mathrm{v} \cdot \exp\left(\frac{\frac{\mathrm{E}}{\mathrm{R}} \cdot (\mathrm{T2} - \mathrm{T1})}{\mathrm{T1} \cdot \mathrm{T2}}\right)}{\mathrm{k} + \mathrm{S}^{\mathrm{h}}} \tag{16}$$

Table 12: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
v	v		2.6		☑
k	k		0.4		☑
h	h		2.0		☑

8.3 Reaction re14

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

Name C3_mRNADegr

SBO:0000179 degradation

Reaction equation

$$\mathrm{s9} \longrightarrow \mathrm{species\_12} \tag{17}$$

Reactant

Table 13: Properties of each reactant.

Id	Name	SBO
s9	C3_mRNA	

Product

Table 14: Properties of each product.

Id	Name	SBO
species_12	junk	

Id	Name	SBO

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \mathrm{vol}\,(\mathrm{default}) \cdot \mathrm{function\_3}\,(\mathrm{v}, \mathrm{parameter\_6}, \mathrm{parameter\_3}, \mathrm{T2}, \mathrm{T}, [\mathrm{s9}], \mathrm{Km}) \tag{18}$$

$$\mathrm{function\_3}\,(\mathrm{v}, \mathrm{E}, \mathrm{R}, \mathrm{T2}, \mathrm{T1}, \mathrm{S}, \mathrm{Km}) = \frac{\mathrm{v} \cdot \exp\left(\frac{\frac{\mathrm{E}}{\mathrm{R}} \cdot (\mathrm{T2} - \mathrm{T1})}{\mathrm{T1} \cdot \mathrm{T2}}\right) \cdot \mathrm{S}}{\mathrm{Km} + \mathrm{S}} \tag{19}$$

$$\mathrm{function\_3}\,(\mathrm{v}, \mathrm{E}, \mathrm{R}, \mathrm{T2}, \mathrm{T1}, \mathrm{S}, \mathrm{Km}) = \frac{\mathrm{v} \cdot \exp\left(\frac{\frac{\mathrm{E}}{\mathrm{R}} \cdot (\mathrm{T2} - \mathrm{T1})}{\mathrm{T1} \cdot \mathrm{T2}}\right) \cdot \mathrm{S}}{\mathrm{Km} + \mathrm{S}} \tag{20}$$

Table 15: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
v	v		3.0		☑
Km	Km		2.0		☑

8.4 Reaction re15

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

Name C3_degr

SBO:0000179 degradation

Reaction equation

$$\mathrm{s10} \longrightarrow \mathrm{species\_12} \tag{21}$$

Reactant

Table 16: Properties of each reactant.

Id	Name	SBO
s10	C_3	

Product

Table 17: Properties of each product.

Id	Name	SBO
species_12	junk	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \mathrm{vol}\,(\mathrm{default}) \cdot \mathrm{function\_3}\,(\mathrm{v}, \mathrm{parameter\_6}, \mathrm{parameter\_3}, \mathrm{T2}, \mathrm{T}, [\mathrm{s10}], \mathrm{Km}) \tag{22}$$

$$\mathrm{function\_3}\,(\mathrm{v}, \mathrm{E}, \mathrm{R}, \mathrm{T2}, \mathrm{T1}, \mathrm{S}, \mathrm{Km}) = \frac{\mathrm{v} \cdot \exp\left(\frac{\frac{\mathrm{E}}{\mathrm{R}} \cdot (\mathrm{T2} - \mathrm{T1})}{\mathrm{T1} \cdot \mathrm{T2}}\right) \cdot \mathrm{S}}{\mathrm{Km} + \mathrm{S}} \tag{23}$$

$$\mathrm{function\_3}\,(\mathrm{v}, \mathrm{E}, \mathrm{R}, \mathrm{T2}, \mathrm{T1}, \mathrm{S}, \mathrm{Km}) = \frac{\mathrm{v} \cdot \exp\left(\frac{\frac{\mathrm{E}}{\mathrm{R}} \cdot (\mathrm{T2} - \mathrm{T1})}{\mathrm{T1} \cdot \mathrm{T2}}\right) \cdot \mathrm{S}}{\mathrm{Km} + \mathrm{S}} \tag{24}$$

Table 18: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
v	v		2.2		☑
Km	Km		0.2		☑

8.5 Reaction re16

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

Name C3_phos_degr

SBO:0000179 degradation

Reaction equation

$$\mathrm{s11} \longrightarrow \mathrm{species\_12} \tag{25}$$

Reactant

Table 19: Properties of each reactant.

Id	Name	SBO
s11	C_3_P	

Product

Table 20: Properties of each product.

Id	Name	SBO
species_12	junk	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \mathrm{vol}\,(\mathrm{default}) \cdot \mathrm{function\_3}\,(\mathrm{v}, \mathrm{parameter\_6}, \mathrm{parameter\_3}, \mathrm{T2}, \mathrm{T}, [\mathrm{s11}], \mathrm{Km}) \tag{26}$$

$$\mathrm{function\_3}\,(\mathrm{v}, \mathrm{E}, \mathrm{R}, \mathrm{T2}, \mathrm{T1}, \mathrm{S}, \mathrm{Km}) = \frac{\mathrm{v} \cdot \exp\left(\frac{\frac{\mathrm{E}}{\mathrm{R}} \cdot (\mathrm{T2} - \mathrm{T1})}{\mathrm{T1} \cdot \mathrm{T2}}\right) \cdot \mathrm{S}}{\mathrm{Km} + \mathrm{S}} \tag{27}$$

$$\mathrm{function\_3}\,(\mathrm{v}, \mathrm{E}, \mathrm{R}, \mathrm{T2}, \mathrm{T1}, \mathrm{S}, \mathrm{Km}) = \frac{\mathrm{v} \cdot \exp\left(\frac{\frac{\mathrm{E}}{\mathrm{R}} \cdot (\mathrm{T2} - \mathrm{T1})}{\mathrm{T1} \cdot \mathrm{T2}}\right) \cdot \mathrm{S}}{\mathrm{Km} + \mathrm{S}} \tag{28}$$

Table 21: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
v	v		1.5		☑
Km	Km		1.4		☑

8.6 Reaction re18

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

Name C3_transl

SBO:0000184 translation

Reaction equation

$$\mathrm{s13} \xrightarrow{\mathrm{s9}} \mathrm{s10} \tag{29}$$

Reactant

Table 22: Properties of each reactant.

Id	Name	SBO
s13	C_3_pre	

Modifier

Table 23: Properties of each modifier.

Id	Name	SBO
s9	C3_mRNA	

Product

Table 24: Properties of each product.

Id	Name	SBO
s10	C_3	

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \mathrm{vol}\left(\mathrm{default}\right) \cdot \mathrm{function\_4}\left(\mathrm{v}, \mathrm{parameter\_7}, \mathrm{parameter\_3}, \mathrm{T2}, \mathrm{T}, \left[\mathrm{s9}\right]\right) \tag{30}$$

$$\mathrm{function\_4}\left(\mathrm{v}, \mathrm{E}, \mathrm{R}, \mathrm{T2}, \mathrm{T1}, \mathrm{S}\right) = \mathrm{v} \cdot \exp\left(\frac{\frac{\mathrm{E}}{\mathrm{R}} \cdot \left(\mathrm{T2} - \mathrm{T1}\right)}{\mathrm{T1} \cdot \mathrm{T2}}\right) \cdot \mathrm{S} \tag{31}$$

$$\mathrm{function\_4}\left(\mathrm{v}, \mathrm{E}, \mathrm{R}, \mathrm{T2}, \mathrm{T1}, \mathrm{S}\right) = \mathrm{v} \cdot \exp\left(\frac{\frac{\mathrm{E}}{\mathrm{R}} \cdot \left(\mathrm{T2} - \mathrm{T1}\right)}{\mathrm{T1} \cdot \mathrm{T2}}\right) \cdot \mathrm{S} \tag{32}$$

Table 25: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
v	v		5.0		☑

8.7 Reaction `reaction_1`

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

Name C1_transl

SBO:0000184 translation

Reaction equation

$$\text{species\_2} \longrightarrow \text{species\_1} \tag{33}$$

Reactant

Table 26: Properties of each reactant.

Id	Name	SBO
`species_2`	C1_mRNA	

Product

Table 27: Properties of each product.

Id	Name	SBO
`species_1`	C1	

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \text{vol}\left(\text{default}\right) \cdot \text{function\_1}\left(\text{v}, \text{E}, \text{parameter\_3}, \text{T2}, \text{T}, [\text{species\_2}]\right) \tag{34}$$

$$\text{function\_1}\left(\text{v}, \text{E}, \text{R}, \text{T2}, \text{T1}, \text{S}\right) = \text{v} \cdot \exp\left(\frac{\frac{\text{E}}{\text{R}} \cdot \left(\text{T2} - \text{T1}\right)}{\text{T1} \cdot \text{T2}}\right) \cdot \text{S} \tag{35}$$

$$\text{function\_1}\left(\text{v}, \text{E}, \text{R}, \text{T2}, \text{T1}, \text{S}\right) = \text{v} \cdot \exp\left(\frac{\frac{\text{E}}{\text{R}} \cdot \left(\text{T2} - \text{T1}\right)}{\text{T1} \cdot \text{T2}}\right) \cdot \text{S} \tag{36}$$

Table 28: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
v	v		19.0		☑
E	E		67000.0		☑

8.8 Reaction `reaction_2`

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

Name complexformation

SBO:0000526 protein complex formation

Reaction equation

$$\text{species\_3} + \text{s11} \longrightarrow \text{species\_4} \tag{37}$$

Reactants

Table 29: Properties of each reactant.

Id	Name	SBO
`species_3`	C1_phos	
`s11`	C_3_P	

Product

Table 30: Properties of each product.

Id	Name	SBO
`species_4`	c1c3complex	

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \text{vol}(\text{default}) \cdot \text{function\_5}(\text{v}, \text{parameter\_7}, \text{parameter\_3}, \text{T2}, \text{T}, [\text{species\_3}], [\text{s11}], \text{a}) \tag{38}$$

$$\text{function\_5}(\text{v}, \text{E}, \text{R}, \text{T2}, \text{T1}, \text{S1}, \text{S2}, \text{a}) = \text{v} \cdot \exp\left(\frac{\frac{\text{E}}{\text{R}} \cdot (\text{T2} - \text{T1})}{\text{T1} \cdot \text{T2}}\right) \cdot \text{S1} \cdot \text{S2}^{\text{a}} \tag{39}$$

$$\text{function\_5}\left(\text{v},\text{E},\text{R},\text{T2},\text{T1},\text{S1},\text{S2},\text{a}\right) = \text{v}\cdot\exp\left(\frac{\frac{\text{E}}{\text{R}}\cdot\left(\text{T2}-\text{T1}\right)}{\text{T1}\cdot\text{T2}}\right)\cdot\text{S1}\cdot\text{S2}^{\text{a}} \tag{40}$$

Table 31: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
v	v		10.0		☑
a	a		2.0		☑

8.9 Reaction `reaction_3`

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

Name C1_phos

SBO:0000216 phosphorylation

Reaction equation

$$\text{species\_1} \longrightarrow \text{species\_3} \tag{41}$$

Reactant

Table 32: Properties of each reactant.

Id	Name	SBO
`species_1`	C1	

Product

Table 33: Properties of each product.

Id	Name	SBO
`species_3`	C1_phos	

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \text{vol}\left(\text{default}\right)\cdot\text{function\_1}\left(\text{parameter\_1},\text{parameter\_9},\text{parameter\_3},\text{T2},\text{T},[\text{species\_1}]\right) \tag{42}$$

$$\text{function\_1}\left(\text{v},\text{E},\text{R},\text{T2},\text{T1},\text{S}\right) = \text{v} \cdot \exp\left(\frac{\frac{\text{E}}{\text{R}} \cdot \left(\text{T2} - \text{T1}\right)}{\text{T1} \cdot \text{T2}}\right) \cdot \text{S} \tag{43}$$

$$\text{function\_1}\left(\text{v},\text{E},\text{R},\text{T2},\text{T1},\text{S}\right) = \text{v} \cdot \exp\left(\frac{\frac{\text{E}}{\text{R}} \cdot \left(\text{T2} - \text{T1}\right)}{\text{T1} \cdot \text{T2}}\right) \cdot \text{S} \tag{44}$$

8.10 Reaction `reaction_4`

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

Name C1_degr

SBO:0000179 degradation

Reaction equation

$$\text{species\_1} \longrightarrow \text{species\_12} \tag{45}$$

Reactant

Table 34: Properties of each reactant.

Id	Name	SBO
`species_1`	C1	

Product

Table 35: Properties of each product.

Id	Name	SBO
`species_12`	junk	

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = \text{vol}\left(\text{default}\right) \cdot \text{function\_3}\left(\text{v},\text{E},\text{parameter\_3},\text{T2},\text{T},\left[\text{species\_1}\right],\text{Km}\right) \tag{46}$$

$$\text{function\_3}\left(\text{v},\text{E},\text{R},\text{T2},\text{T1},\text{S},\text{Km}\right) = \frac{\text{v} \cdot \exp\left(\frac{\frac{\text{E}}{\text{R}} \cdot \left(\text{T2}-\text{T1}\right)}{\text{T1} \cdot \text{T2}}\right) \cdot \text{S}}{\text{Km} + \text{S}} \tag{47}$$

$$\text{function\_3}\left(\text{v},\text{E},\text{R},\text{T2},\text{T1},\text{S},\text{Km}\right) = \frac{\text{v}\cdot\exp\left(\frac{\frac{\text{E}}{\text{R}}\cdot\left(\text{T2}-\text{T1}\right)}{\text{T1}\cdot\text{T2}}\right)\cdot\text{S}}{\text{Km}+\text{S}} \tag{48}$$

Table 36: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
v	v		30.0		☑
E	E		67000.0		☑
Km	Km		2.0		☑

8.11 Reaction reaction_5

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

Name complexdegr

SBO:0000179 degradation

Reaction equation

$$\text{species\_4} \longrightarrow \text{species\_12} \tag{49}$$

Reactant

Table 37: Properties of each reactant.

Id	Name	SBO
species_4	c1c3complex	

Product

Table 38: Properties of each product.

Id	Name	SBO
species_12	junk	

Kinetic Law

Derived unit contains undeclared units

$$v_{11} = \text{vol}\left(\text{default}\right)\cdot\text{function\_3}\left(\text{v},\text{E},\text{parameter\_3},\text{T2},\text{T},\left[\text{species\_4}\right],\text{Km}\right) \tag{50}$$

$$\text{function\_3}\left(\text{v},\text{E},\text{R},\text{T2},\text{T1},\text{S},\text{Km}\right) = \frac{\text{v}\cdot\exp\left(\frac{\frac{\text{E}}{\text{R}}\cdot\left(\text{T2}-\text{T1}\right)}{\text{T1}\cdot\text{T2}}\right)\cdot\text{S}}{\text{Km}+\text{S}} \tag{51}$$

$$\text{function\_3}\left(\text{v},\text{E},\text{R},\text{T2},\text{T1},\text{S},\text{Km}\right) = \frac{\text{v}\cdot\exp\left(\frac{\frac{\text{E}}{\text{R}}\cdot\left(\text{T2}-\text{T1}\right)}{\text{T1}\cdot\text{T2}}\right)\cdot\text{S}}{\text{Km}+\text{S}} \tag{52}$$

Table 39: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
v	v		20.0		☑
E	E		67000.0		☑
Km	Km		4.0		☑

8.12 Reaction reaction_6

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

Name C1_dephos

SBO:0000330 dephosphorylation

Reaction equation

$$\text{species\_3} \longrightarrow \text{species\_1} \tag{53}$$

Reactant

Table 40: Properties of each reactant.

Id	Name	SBO
species_3	C1_phos	

Product

Table 41: Properties of each product.

Id	Name	SBO
species_1	C1	

Kinetic Law

Derived unit contains undeclared units

$$v_{12} = \mathrm{vol}\left(\mathrm{default}\right) \cdot \mathrm{function\_1}\left(\mathrm{parameter\_2}, \mathrm{parameter\_10}, \mathrm{parameter\_3}, \mathrm{T2}, \mathrm{T}, \left[\mathrm{species\_3}\right]\right) \tag{54}$$

$$\mathrm{function\_1}\left(\mathrm{v}, \mathrm{E}, \mathrm{R}, \mathrm{T2}, \mathrm{T1}, \mathrm{S}\right) = \mathrm{v} \cdot \exp\left(\frac{\frac{\mathrm{E}}{\mathrm{R}} \cdot \left(\mathrm{T2} - \mathrm{T1}\right)}{\mathrm{T1} \cdot \mathrm{T2}}\right) \cdot \mathrm{S} \tag{55}$$

$$\mathrm{function\_1}\left(\mathrm{v}, \mathrm{E}, \mathrm{R}, \mathrm{T2}, \mathrm{T1}, \mathrm{S}\right) = \mathrm{v} \cdot \exp\left(\frac{\frac{\mathrm{E}}{\mathrm{R}} \cdot \left(\mathrm{T2} - \mathrm{T1}\right)}{\mathrm{T1} \cdot \mathrm{T2}}\right) \cdot \mathrm{S} \tag{56}$$

8.13 Reaction `reaction_7`

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

Name C1_phos_degr

SBO:0000179 degradation

Reaction equation

$$\mathrm{species\_3} \longrightarrow \mathrm{species\_12} \tag{57}$$

Reactant

Table 42: Properties of each reactant.

Id	Name	SBO
`species_3`	C1_phos	

Product

Table 43: Properties of each product.

Id	Name	SBO
`species_12`	junk	

Kinetic Law

Derived unit contains undeclared units

$$v_{13} = \mathrm{vol}\,(\mathrm{default}) \cdot \mathrm{function\_3}\,(\mathrm{parameter\_8}, \mathrm{E}, \mathrm{parameter\_3}, \mathrm{T2}, \mathrm{T}, [\mathrm{species\_3}], \mathrm{Km}) \quad (58)$$

$$\mathrm{function\_3}\,(\mathrm{v}, \mathrm{E}, \mathrm{R}, \mathrm{T2}, \mathrm{T1}, \mathrm{S}, \mathrm{Km}) = \frac{\mathrm{v} \cdot \exp\left(\frac{\frac{\mathrm{E}}{\mathrm{R}} \cdot (\mathrm{T2} - \mathrm{T1})}{\mathrm{T1} \cdot \mathrm{T2}}\right) \cdot \mathrm{S}}{\mathrm{Km} + \mathrm{S}} \quad (59)$$

$$\mathrm{function\_3}\,(\mathrm{v}, \mathrm{E}, \mathrm{R}, \mathrm{T2}, \mathrm{T1}, \mathrm{S}, \mathrm{Km}) = \frac{\mathrm{v} \cdot \exp\left(\frac{\frac{\mathrm{E}}{\mathrm{R}} \cdot (\mathrm{T2} - \mathrm{T1})}{\mathrm{T1} \cdot \mathrm{T2}}\right) \cdot \mathrm{S}}{\mathrm{Km} + \mathrm{S}} \quad (60)$$

Table 44: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
E	E		67000.0		☑
Km	Km		1.0		☑

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 s2

Name C3_Gene

SBO:0000243 gene

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

This species takes part in one reaction (as a reactant in re13), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s2} = 0 \quad (61)$$

9.2 Species s9

Name C3_mRNA

SBO:0000278 messenger RNA

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

This species takes part in three reactions (as a reactant in re14 and as a product in re13 and as a modifier in re18).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s9} = v_2 - v_3 \tag{62}$$

9.3 Species s10

Name C_3

SBO:0000252 polypeptide chain

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

This species takes part in three reactions (as a reactant in re12, re15 and as a product in re18).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s10} = v_6 - v_1 - v_4 \tag{63}$$

9.4 Species s11

Name C_3_P

SBO:0000252 polypeptide chain

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

This species takes part in four reactions (as a reactant in re16, reaction_2 and as a product in re12 and as a modifier in re13).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s11} = v_1 - v_5 - v_8 \tag{64}$$

9.5 Species s13

Name C_3_pre

SBO:0000252 polypeptide chain

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

This species takes part in one reaction (as a reactant in re18), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s13} = 0 \tag{65}$$

9.6 Species species_1

Name C1

SBO:0000252 polypeptide chain

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

This species takes part in four reactions (as a reactant in reaction_3, reaction_4 and as a product in reaction_1, reaction_6).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_1} = v_7 + v_{12} - v_9 - v_{10} \tag{66}$$

9.7 Species species_2

Name C1_mRNA

SBO:0000278 messenger RNA

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

This species takes part in one reaction (as a reactant in reaction_1), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_2} = 0 \tag{67}$$

9.8 Species species_3

Name C1_phos

SBO:0000252 polypeptide chain

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

This species takes part in four reactions (as a reactant in reaction_2, reaction_6, reaction_7 and as a product in reaction_3).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_3} = v_9 - v_8 - v_{12} - v_{13} \tag{68}$$

9.9 Species species_4

Name c1c3complex

SBO:0000297 protein complex

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

This species takes part in two reactions (as a reactant in reaction_5 and as a product in reaction_2).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_4} = v_8 - v_{11} \tag{69}$$

9.10 Species species_12

Name junk

SBO:0000291 empty set

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

This species takes part in six reactions (as a product in re14, re15, re16, reaction_4, reaction_5, reaction_7).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{species\_12} = v_3 + v_4 + v_5 + v_{10} + v_{11} + v_{13} \tag{70}$$

A Glossary of Systems Biology Ontology Terms

SBO:0000147 thermodynamic temperature: Temperature is the physical property of a system which underlies the common notions of“ho” and“col”; the material with the higher temperature is said to be hotter. Temperature is a quantity related to the average kinetic energy of the particles in a substance. The 10th Conference Generale des Poids et Mesures decided to define the thermodynamic temperature scale by choosing the triple point of water as the fundamental fixed point, and assigning to it the temperature 273,16 degrees Kelvin, exactly (0.01 degree Celsius)

SBO:0000179 degradation: Complete disappearance of a physical entity

SBO:0000183 transcription: Process through which a DNA sequence is copied to produce a complementary RNA

SBO:0000184 translation: Process in which a polypeptide chain is produced from a messenger RNA

SBO:0000216 phosphorylation: Addition of a phosphate group (-H2PO4) to a chemical entity

SBO:0000243 gene: A locatable region of genomic sequence, corresponding to a unit of inheritance, which is associated with regulatory regions, transcribed regions and/or other functional sequence regions. Sequence Ontology SO:000070

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:0000291 empty set: Entity defined by the absence of any actual object. An empty set is often used to represent the source of a creation process or the result of a degradation process.

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

SBO:0000330 dephosphorylation: Removal of a phosphate group (-H2PO4) from a chemical entity.

SBO:0000526 protein complex formation: The process by which two or more proteins interact non-covalently to form a protein complex (SBO:0000297)

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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