SBML Model Report

Model name: "Smolen2002_CircClock"

May 5, 2016

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by Nicolas Le Novre[1] at June 29th 2005 at 11:01 a. m. and last time modified at February 25th 2015 at 12:51 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	4
events	0	constraints	0
reactions	4	function definitions	0
global parameters	10	unit definitions	5
rules	3	initial assignments	0

Model Notes

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To cite BioModels Database, please use Le Novre N., Bornstein B., Broicher A., Courtot M., Donizelli M., Dharuri H., Li L., Sauro H., Schilstra M., Shapiro B., Snoep J.L., Hucka M. (2006) BioModels Database: A Free, Centralized Database of Curated, Published, Quantitative Kinetic Models of Biochemical and Cellular Systems Nucleic Acids Res., 34: D689-D691.

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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 `time`

Name hour (new default)

Definition 3600 s

2.2 Unit `substance`

Name nanomole (new default)

Definition nmol

2.3 Unit `nM`

Name nM

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

2.4 Unit `nM_per_hr`

Name nM_per_hr

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

2.5 Unit `per_hr`

Name per_hr

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

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
CELL			3	10^{-15}	l	☑	

3.1 Compartment CELL

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

4 Species

This model contains four 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 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
`EmptySet`		`CELL`	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	☑	☑
`Per`		`CELL`	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	☐	☐
`dClk`		`CELL`	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	☐	☐
`dClkF`	free dClk	`CELL`	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	☐	☐

5 Parameters

This model contains ten global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
dClkF_tau1	dClkF_tau1		0.00	$\mathrm{nmol \cdot l^{-1}}$	⊟
dClkF_tau2	dClkF_tau2		0.00	$\mathrm{nmol \cdot l^{-1}}$	⊟
tau1	tau1		10.00	3600 s	☑
tau2	tau2		10.00	3600 s	☑
Vsp	Vsp		0.50	$\mathrm{nmol \cdot l^{-1} \cdot (3600\ s)^{-1}}$	☑
K1	K1		0.30	$\mathrm{nmol \cdot l^{-1}}$	☑
Vsc	Vsc		0.25	$\mathrm{nmol \cdot l^{-1} \cdot (3600\ s)^{-1}}$	☑
K2	K2		0.10	$\mathrm{nmol \cdot l^{-1}}$	☑
kdc	kdc		0.50	$\mathrm{(3600\ s)^{-1}}$	☑
kdp	kdp		0.50	$\mathrm{(3600\ s)^{-1}}$	☑

6 Rules

This is an overview of three rules.

6.1 Rule dClkF

Rule dClkF is an assignment rule for species dClkF:

$$\mathrm{dClkF} = \begin{cases} 0 & \text{if } [\mathrm{dClk}] - [\mathrm{Per}] < 0 \\ [\mathrm{dClk}] - [\mathrm{Per}] & \text{otherwise} \end{cases} \tag{1}$$

6.2 Rule dClkF_tau1

Rule dClkF_tau1 is an assignment rule for parameter dClkF_tau1:

$$\mathrm{dClkF\_tau1} = \begin{cases} 0 & \text{if } \mathrm{delay} - \mathrm{delay} < 0 \\ \mathrm{delay} - \mathrm{delay} & \text{otherwise} \end{cases} \tag{2}$$

6.3 Rule dClkF_tau2

Rule dClkF_tau2 is an assignment rule for parameter dClkF_tau2:

$$\mathrm{dClkF\_tau2} = \begin{cases} 0 & \text{if } \mathrm{delay} - \mathrm{delay} < 0 \\ \mathrm{delay} - \mathrm{delay} & \text{otherwise} \end{cases} \tag{3}$$

7 Reactions

This model contains four 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	`rPer`	Per production	EmptySet $\xrightarrow{\text{dClkF}}$ Per	
2	`rdClk`	dClk production	EmptySet $\xrightarrow{\text{dClkF}}$ dClk	
3	`rPerD`	Per degradation	Per $\longrightarrow$ EmptySet	
4	`rdClkD`	dClk degradation	dClk $\longrightarrow$ EmptySet	

7.1 Reaction rPer

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

Name Per production

Reaction equation

$$\text{EmptySet} \xrightarrow{\text{dClkF}} \text{Per} \tag{4}$$

Reactant

Table 6: Properties of each reactant.

Id	Name	SBO
EmptySet		

Modifier

Table 7: Properties of each modifier.

Id	Name	SBO
dClkF	free dClk	

Product

Table 8: Properties of each product.

Id	Name	SBO
Per		

Kinetic Law

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

$$v_1 = \text{Vsp} \cdot \frac{\text{dClkF\_tau1}}{\text{K1} + \text{dClkF\_tau1}} \cdot \text{vol}\,(\text{CELL}) \tag{5}$$

7.2 Reaction rdClk

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

Name dClk production

Reaction equation

$$\text{EmptySet} \xrightarrow{\text{dClkF}} \text{dClk} \tag{6}$$

Reactant

Table 9: Properties of each reactant.

Id	Name	SBO
EmptySet		

Modifier

Table 10: Properties of each modifier.

Id	Name	SBO
dClkF	free dClk	

Product

Table 11: Properties of each product.

Id	Name	SBO
dClk		

Kinetic Law

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

$$v_2 = \text{vol}\,(\text{CELL}) \cdot \text{Vsc} \cdot \frac{\text{K2}}{\text{K2} + \text{dClkF\_tau2}} \tag{7}$$

7.3 Reaction rPerD

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

Name Per degradation

Reaction equation

$$\text{Per} \longrightarrow \text{EmptySet} \tag{8}$$

Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
Per		

Product

Table 13: Properties of each product.

Id	Name	SBO
EmptySet		

Kinetic Law

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

$$v_3 = \mathrm{kdc} \cdot [\mathrm{Per}] \cdot \mathrm{vol}(\mathrm{CELL}) \tag{9}$$

7.4 Reaction rdClkD

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

Name dClk degradation

Reaction equation

$$\mathrm{dClk} \longrightarrow \mathrm{EmptySet} \tag{10}$$

Reactant

Table 14: Properties of each reactant.

Id	Name	SBO
dClk		

Product

Table 15: Properties of each product.

Id	Name	SBO
EmptySet		

Kinetic Law

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

$$v_4 = \mathrm{kdp} \cdot [\mathrm{dClk}] \cdot \mathrm{vol}\,(\mathrm{CELL}) \tag{11}$$

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 `EmptySet`

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

This species takes part in four reactions (as a reactant in `rPer`, `rdClk` and as a product in `rPerD`, `rdClkD`), which do not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{EmptySet} = 0 \tag{12}$$

8.2 Species `Per`

Initial concentration $5 \cdot 10^{-16}\ \mathrm{nmol} \cdot \mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in `rPerD` and as a product in `rPer`).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Per} = v_1 - v_3 \tag{13}$$

8.3 Species `dClk`

Initial concentration $10^{-16}\ \mathrm{nmol} \cdot \mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in `rdClkD` and as a product in `rdClk`).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{dClk} = v_2 - v_4 \tag{14}$$

8.4 Species `dClkF`

Name free dClk

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

Involved in rule `dClkF`

This species takes part in two reactions (as a modifier in `rPer`, `rdClk`) and is also involved in one rule which determines this species' quantity.

SBML2LaTeX was developed by Andreas Dräger[a], Hannes Planatscher[a], Dieudonné M Wouamba[a], Adrian Schröder[a], Michael Hucka[b], Lukas Endler[c], Martin Golebiewski[d] and Andreas Zell[a]. Please see http://www.ra.cs.uni-tuebingen.de/software/SBML2LaTeX for more information.

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