SBML Model Report

Model name: "Romond1999_CellCycle"

May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 3 format. This model was created by Harish Dharuri[1] at September tenth 2008 at 1:58 p. m. and last time modified at July fifth 2012 at 4:48 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	6	function definitions	0
global parameters	32	unit definitions	5
rules	8	initial assignments	0

Model Notes

The model reproduces Fig 3 of the paper. Model successfully reproduced using MathSBML and Jarnac.

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commercially or not, in a restricted way or not.

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 nine unit definitions of which four are predefined by SBML and not mentioned in the model.

2.1 Unit `time`

Name minute

Definition 60 s

2.2 Unit `uM`

Name uM

Definition $\mu\text{mol} \cdot 1^{-1}$

2.3 Unit `micromole`

Name micromole

Definition μmol

2.4 Unit `min_1`

Name min_1

Definition $(60\ \text{s})^{-1}$

2.5 Unit `uM_min_1`

Name uM_min_1

Definition $\mu\text{mol} \cdot 1^{-1} \cdot (60\ \text{s})^{-1}$

2.6 Unit `substance`

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

Definition mol

2.7 Unit volume

Notes Litre is the predefined SBML unit for volume.

Definition l

2.8 Unit area

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

Definition m^2

2.9 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
compartment			3	1	litre	☑	

3.1 Compartment compartment

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

4 Species

This model contains six 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
C1	cyclinB	compartment	$\mu mol \cdot l^{-1}$	⊟	⊟
M1	cdk1	compartment	dimensionless	⊟	⊟
X1	ubiquitin ligase	compartment	dimensionless	⊟	⊟
C2	cyclinE	compartment	$\mu mol \cdot l^{-1}$	⊟	⊟
M2	cdk2	compartment	dimensionless	⊟	⊟
X2	Ubiquitin ligase 2	compartment	dimensionless	⊟	⊟

5 Parameters

This model contains 32 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
V1			0.000	$(60\ \mathrm{s})^{-1}$	⊟
Kc1			0.500	$\mu\mathrm{mol}\cdot\mathrm{l}^{-1}$	☑
V_M1			0.300	$(60\ \mathrm{s})^{-1}$	☑
V3			0.000	$(60\ \mathrm{s})^{-1}$	⊟
V_M3			0.100	$(60\ \mathrm{s})^{-1}$	☑
U1			0.000	$(60\ \mathrm{s})^{-1}$	⊟
Kc2			0.500	$\mu\mathrm{mol}\cdot\mathrm{l}^{-1}$	☑
U_M1			0.300	$(60\ \mathrm{s})^{-1}$	☑
U3			0.000	$(60\ \mathrm{s})^{-1}$	⊟
U_M3			0.100	$(60\ \mathrm{s})^{-1}$	☑
vi1			0.050	$\mu\mathrm{mol}\cdot\mathrm{l}^{-1}\cdot(60\ \mathrm{s})^{-1}$	☑
Kim1			0.030	dimensionless	☑
vd1			0.025	$\mu\mathrm{mol}\cdot\mathrm{l}^{-1}\cdot(60\ \mathrm{s})^{-1}$	☑
K_d1			0.020	$\mu\mathrm{mol}\cdot\mathrm{l}^{-1}$	☑
kd1			0.001	$(60\ \mathrm{s})^{-1}$	☑
K1			0.010	dimensionless	☑
V2			0.150	$(60\ \mathrm{s})^{-1}$	☑
K2			0.010	dimensionless	☑
K3			0.010	dimensionless	☑
V4			0.050	$(60\ \mathrm{s})^{-1}$	☑
K4			0.010	dimensionless	☑
vi2			0.050	$\mu\mathrm{mol}\cdot\mathrm{l}^{-1}\cdot(60\ \mathrm{s})^{-1}$	☑
Kim2			0.030	dimensionless	☑
vd2			0.025	$\mu\mathrm{mol}\cdot\mathrm{l}^{-1}\cdot(60\ \mathrm{s})^{-1}$	☑
K_d2			0.020	$\mu\mathrm{mol}\cdot\mathrm{l}^{-1}$	☑
kd2			0.001	$(60\ \mathrm{s})^{-1}$	☑
H1			0.010	dimensionless	☑
U2			0.150	$(60\ \mathrm{s})^{-1}$	☑
H2			0.010	dimensionless	☑
H3			0.010	dimensionless	☑
U4			0.050	$(60\ \mathrm{s})^{-1}$	☑
H4			0.010	dimensionless	☑

6 Rules

This is an overview of eight rules.

6.1 Rule `V1`

Rule `V1` is an assignment rule for parameter `V1`:

$$\mathrm{V1} = \frac{[\mathrm{C1}]}{\mathrm{Kc1} + [\mathrm{C1}]} \cdot \mathrm{V\_M1} \tag{1}$$

Derived unit $(60\ \mathrm{s})^{-1}$

6.2 Rule `V3`

Rule `V3` is an assignment rule for parameter `V3`:

$$\mathrm{V3} = \mathrm{M1} \cdot \mathrm{V\_M3} \tag{2}$$

Derived unit $(60\ \mathrm{s})^{-1}$

6.3 Rule `U1`

Rule `U1` is an assignment rule for parameter `U1`:

$$\mathrm{U1} = \frac{[\mathrm{C2}]}{\mathrm{Kc2} + [\mathrm{C2}]} \cdot \mathrm{U\_M1} \tag{3}$$

Derived unit $(60\ \mathrm{s})^{-1}$

6.4 Rule `U3`

Rule `U3` is an assignment rule for parameter `U3`:

$$\mathrm{U3} = \mathrm{M2} \cdot \mathrm{U\_M3} \tag{4}$$

Derived unit $(60\ \mathrm{s})^{-1}$

6.5 Rule `M1`

Rule `M1` is a rate rule for species `M1`:

$$\frac{\mathrm{d}}{\mathrm{d}t}[\mathrm{M1}] = \frac{\mathrm{V1} \cdot (1 - \mathrm{M1})}{\mathrm{K1} + (1 - \mathrm{M1})} - \frac{\mathrm{V2} \cdot \mathrm{M1}}{\mathrm{K2} + \mathrm{M1}} \tag{5}$$

6.6 Rule X1

Rule X1 is a rate rule for species X1:

$$\frac{\mathrm{d}}{\mathrm{d}t}[\mathrm{X1}] = \frac{\mathrm{V3} \cdot (1 - \mathrm{X1})}{\mathrm{K3} + (1 - \mathrm{X1})} - \frac{\mathrm{V4} \cdot \mathrm{X1}}{\mathrm{K4} + \mathrm{X1}} \tag{6}$$

6.7 Rule M2

Rule M2 is a rate rule for species M2:

$$\frac{\mathrm{d}}{\mathrm{d}t}[\mathrm{M2}] = \frac{\mathrm{U1} \cdot (1 - \mathrm{M2})}{\mathrm{H1} + (1 - \mathrm{M2})} - \frac{\mathrm{U2} \cdot \mathrm{M2}}{\mathrm{H2} + \mathrm{M2}} \tag{7}$$

6.8 Rule X2

Rule X2 is a rate rule for species X2:

$$\frac{\mathrm{d}}{\mathrm{d}t}[\mathrm{X2}] = \frac{\mathrm{U3} \cdot (1 - \mathrm{X2})}{\mathrm{H3} + (1 - \mathrm{X2})} - \frac{\mathrm{U4} \cdot \mathrm{X2}}{\mathrm{H4} + \mathrm{X2}} \tag{8}$$

7 Reactions

This model contains six 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	cdk2 mediated cyclinB synthesis	$\emptyset \xrightarrow{M2} C1$	
2	R2	Ubiquitin ligase mediated cyclinB degradation	$C1 \xrightarrow{X1} \emptyset$	
3	R3	cyclinB degradation	$C1 \longrightarrow \emptyset$	
4	R8	cyclinE synthesis	$\emptyset \xrightarrow{M1} C2$	
5	R9	Ubiquitin ligase mediated cyclinE degradation	$C2 \xrightarrow{X2} \emptyset$	
6	R10	cyclinE degradation	$C2 \longrightarrow \emptyset$	

7.1 Reaction R1

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

Name cdk2 mediated cyclinB synthesis

Reaction equation

$$\emptyset \xrightarrow{\mathrm{M2}} \mathrm{C1} \tag{9}$$

Modifier

Table 6: Properties of each modifier.

Id	Name	SBO
M2	cdk2	

Product

Table 7: Properties of each product.

Id	Name	SBO
C1	cyclinB	

Kinetic Law

Derived unit $\mu\mathrm{mol} \cdot (60\ \mathrm{s})^{-1}$

$$v_1 = \frac{\mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{vi1} \cdot \mathrm{Kim1}}{\mathrm{Kim1} + \mathrm{M2}} \tag{10}$$

7.2 Reaction R2

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

Name Ubiquitin ligase mediated cyclinB degradation

Reaction equation

$$\mathrm{C1} \xrightarrow{\mathrm{X1}} \emptyset \tag{11}$$

Reactant

Table 8: Properties of each reactant.

Id	Name	SBO
C1	cyclinB	

Modifier

Table 9: Properties of each modifier.

Id	Name	SBO
X1	ubiquitin ligase	

Kinetic Law

Derived unit $10^{-6}\ \mathrm{mol} \cdot (60\ \mathrm{s})^{-1}$

$$v_2 = \frac{\mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{vd1} \cdot \mathrm{X1} \cdot [\mathrm{C1}]}{\mathrm{K\_d1} + [\mathrm{C1}]} \tag{12}$$

7.3 Reaction R3

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

Name cyclinB degradation

Reaction equation

$$\mathrm{C1} \longrightarrow \emptyset \tag{13}$$

Reactant

Table 10: Properties of each reactant.

Id	Name	SBO
C1	cyclinB	

Kinetic Law

Derived unit $(60\ \mathrm{s})^{-1} \cdot \mu\mathrm{mol}$

$$v_3 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{kd1} \cdot [\mathrm{C1}] \tag{14}$$

7.4 Reaction R8

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

Name cyclinE synthesis

Reaction equation

$$\emptyset \xrightarrow{\mathrm{M1}} \mathrm{C2} \tag{15}$$

Modifier

Table 11: Properties of each modifier.

Id	Name	SBO
M1	cdk1	

Product

Table 12: Properties of each product.

Id	Name	SBO
C2	cyclinE	

Kinetic Law

Derived unit $\mu\mathrm{mol} \cdot (60\ \mathrm{s})^{-1}$

$$v_4 = \frac{\mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{vi2} \cdot \mathrm{Kim2}}{\mathrm{Kim2} + \mathrm{M1}} \tag{16}$$

7.5 Reaction R9

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

Name Ubiquitin ligase mediated cyclinE degradation

Reaction equation

$$\mathrm{C2} \xrightarrow{\mathrm{X2}} \emptyset \tag{17}$$

Reactant

Table 13: Properties of each reactant.

Id	Name	SBO
C2	cyclinE	

Modifier

Table 14: Properties of each modifier.

Id	Name	SBO
X2	Ubiquitin ligase 2	

Kinetic Law

Derived unit $10^{-6}\ \mathrm{mol} \cdot (60\ \mathrm{s})^{-1}$

$$v_5 = \frac{\mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{vd2} \cdot \mathrm{X2} \cdot [\mathrm{C2}]}{\mathrm{K\_d2} + [\mathrm{C2}]} \tag{18}$$

7.6 Reaction R10

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

Name cyclinE degradation

Reaction equation

$$\mathrm{C2} \longrightarrow \emptyset \tag{19}$$

Reactant

Table 15: Properties of each reactant.

Id	Name	SBO
C2	cyclinE	

Kinetic Law

Derived unit $(60\ \mathrm{s})^{-1} \cdot \mu\mathrm{mol}$

$$v_6 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{kd2} \cdot [\mathrm{C2}] \tag{20}$$

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 C1

Name cyclinB

Initial concentration $2\ \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in three reactions (as a reactant in R2, R3 and as a product in R1).

$$\frac{\text{d}}{\text{d}t}\text{C1} = v_1 - v_2 - v_3 \tag{21}$$

8.2 Species M1

Name cdk1

Initial amount 1 dimensionless

Involved in rule M1

This species takes part in one reaction (as a modifier in R8) and is also involved in one rule which determines this species' quantity.

8.3 Species X1

Name ubiquitin ligase

Initial amount 0 dimensionless

Involved in rule X1

This species takes part in one reaction (as a modifier in R2) and is also involved in one rule which determines this species' quantity.

8.4 Species C2

Name cyclinE

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

This species takes part in three reactions (as a reactant in R9, R10 and as a product in R8).

$$\frac{\text{d}}{\text{d}t}\text{C2} = v_4 - v_5 - v_6 \tag{22}$$

8.5 Species M2

Name cdk2

Initial amount 0 dimensionless

Involved in rule M2

This species takes part in one reaction (as a modifier in R1) and is also involved in one rule which determines this species' quantity.

8.6 Species X2

Name Ubiquitin ligase 2

Initial amount 0 dimensionless

Involved in rule X2

This species takes part in one reaction (as a modifier in R9) 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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