SBML Model Report

Model name: "Deineko2003_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 thirteenth 2008 at 5:21 a. m. and last time modified at July fifth 2012 at 2:41 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	15	function definitions	0
global parameters	18	unit definitions	0
rules	1	initial assignments	0

Model Notes

The model reproduces Fig 3 of the paper corresponding to the transition to S phase. Units have not been defined for this model because the paper mentions the use of arbitrary units for the various species and parameters. Model reproduced using MathSBML.

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In summary, you are entitled to use this encoded model in absolutely any manner you deem suitable, verbatim, or with modification, alone or embedded it in a larger context, redistribute it, 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 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
`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
y1	E2F	compartment	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
y2	pRB	compartment	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
y3	Phosphorylated pRB	compartment	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
y4	inactive cycE_cdk2	compartment	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
y5	active cycE_cdk2	compartment	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
y6	AP-1	compartment	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟

5 Parameters

This model contains 18 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
emax			2.000		☑
k1			1.000		☑
k1_prime			1.000		☑
k1_double-_prime			10.000		☑
phi1			0.100		☑
k2			1.000		☑
k3			0.400		☑
phi2			0.010		☑
phi3			0.100		☑
k4			0.090		☑
k4_double-_prime			0.100		☑
k4i			1.000		☑
k4a			2.000		☑
phi4i			0.010		☑
phi4a			0.010		☑
k6			0.000		☑
F6			0.044		☐
phi6			0.100		☑

6 Rule

This is an overview of one rule.

6.1 Rule F6

Rule F6 is an assignment rule for parameter F6:

$$\mathrm{F6} = \begin{cases} 0.044 & \text{if } \mathrm{t} \leq 60 \\ 0 & \text{otherwise} \end{cases} \tag{1}$$

7 Reactions

This model contains 15 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		$\emptyset \xrightarrow{y2} y1$	
2	R2		$y1 \longrightarrow \emptyset$	
3	R3		$\emptyset \xrightarrow{y1} y2$	
4	R4		$y2 \xrightarrow{y5} y3$	
5	R5		$y2 \longrightarrow \emptyset$	
6	R6		$y3 \longrightarrow \emptyset$	
7	R7		$\emptyset \xrightarrow{y1} y4$	
8	R8		$\emptyset \xrightarrow{y6} y4$	
9	R9		$y4 \longrightarrow y5$	
10	R10		$y5 \longrightarrow y4$	
11	R11		$y4 \longrightarrow \emptyset$	
12	R12		$y5 \longrightarrow \emptyset$	
13	R13		$\emptyset \xrightarrow{y1} y6$	
14	R14		$\emptyset \longrightarrow y6$	
15	R15		$y6 \longrightarrow \emptyset$	

7.1 Reaction R1

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

Reaction equation

$$\emptyset \xrightarrow{\text{y2}} \text{y1} \tag{2}$$

Modifier

Table 6: Properties of each modifier.

Id	Name	SBO
y2	pRB	

Product

Table 7: Properties of each product.

Id	Name	SBO
y1	E2F	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \frac{\text{emax} \cdot \text{k1} \cdot [\text{y1}]}{\text{k1} \cdot [\text{y1}] + (\text{k1\_prime} + \text{k1\_double\_prime} \cdot [\text{y1}]) \cdot [\text{y2}]} \tag{3}$$

7.2 Reaction R2

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

Reaction equation

$$\text{y1} \longrightarrow \emptyset \tag{4}$$

Reactant

Table 8: Properties of each reactant.

Id	Name	SBO
y1	E2F	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \text{phi1} \cdot [\text{y1}] \tag{5}$$

7.3 Reaction R3

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

Reaction equation

$$\emptyset \xrightarrow{\text{y1}} \text{y2} \tag{6}$$

Modifier

Table 9: Properties of each modifier.

Id	Name	SBO
y1	E2F	

Product

Table 10: Properties of each product.

Id	Name	SBO
y2	pRB	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \text{k2} \cdot [\text{y1}] \tag{7}$$

7.4 Reaction R4

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

Reaction equation

$$\mathrm{y2} \xrightarrow{\mathrm{y5}} \mathrm{y3} \tag{8}$$

Reactant

Table 11: Properties of each reactant.

Id	Name	SBO
y2	pRB	

Modifier

Table 12: Properties of each modifier.

Id	Name	SBO
y5	active cycE_cdk2	

Product

Table 13: Properties of each product.

Id	Name	SBO
y3	Phosphorylated pRB	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \mathrm{k3} \cdot [\mathrm{y2}] \cdot [\mathrm{y5}] \tag{9}$$

7.5 Reaction R5

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

Reaction equation

$$\mathrm{y2} \longrightarrow \emptyset \tag{10}$$

Reactant

Table 14: Properties of each reactant.

Id	Name	SBO
y2	pRB	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \text{phi2} \cdot [\text{y2}] \tag{11}$$

7.6 Reaction R6

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

Reaction equation

$$\text{y3} \longrightarrow \emptyset \tag{12}$$

Reactant

Table 15: Properties of each reactant.

Id	Name	SBO
y3	Phosphorylated pRB	

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \text{phi3} \cdot [\text{y3}] \tag{13}$$

7.7 Reaction R7

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

Reaction equation

$$\emptyset \xrightarrow{\text{y1}} \text{y4} \tag{14}$$

Modifier

Table 16: Properties of each modifier.

Id	Name	SBO
y1	E2F	

Product

Table 17: Properties of each product.

Id	Name	SBO
y4	inactive cycE_cdk2	

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \mathrm{k4} \cdot [\mathrm{y1}] \tag{15}$$

7.8 Reaction R8

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

Reaction equation

$$\emptyset \xrightarrow{\mathrm{y6}} \mathrm{y4} \tag{16}$$

Modifier

Table 18: Properties of each modifier.

Id	Name	SBO
y6	AP-1	

Product

Table 19: Properties of each product.

Id	Name	SBO
y4	inactive cycE_cdk2	

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \text{k4\_double\_prime} \cdot [\text{y6}] \tag{17}$$

7.9 Reaction R9

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

Reaction equation

$$\text{y4} \longrightarrow \text{y5} \tag{18}$$

Reactant

Table 20: Properties of each reactant.

Id	Name	SBO
y4	inactive cycE_cdk2	

Product

Table 21: Properties of each product.

Id	Name	SBO
y5	active cycE_cdk2	

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \text{k4i} \cdot [\text{y4}] \cdot [\text{y5}] \tag{19}$$

7.10 Reaction R10

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

Reaction equation

$$\text{y5} \longrightarrow \text{y4} \tag{20}$$

Reactant

Table 22: Properties of each reactant.

Id	Name	SBO
y5	active cycE_cdk2	

Product

Table 23: Properties of each product.

Id	Name	SBO
y4	inactive cycE_cdk2	

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = \text{k4a} \cdot [\text{y5}] \tag{21}$$

7.11 Reaction R11

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

Reaction equation

$$\text{y4} \longrightarrow \emptyset \tag{22}$$

Reactant

Table 24: Properties of each reactant.

Id	Name	SBO
y4	inactive cycE_cdk2	

Kinetic Law

Derived unit contains undeclared units

$$v_{11} = \text{phi4i} \cdot [\text{y4}] \tag{23}$$

7.12 Reaction R12

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

Reaction equation

$$\mathrm{y5} \longrightarrow \emptyset \tag{24}$$

Reactant

Table 25: Properties of each reactant.

Id	Name	SBO
y5	active cycE_cdk2	

Kinetic Law

Derived unit contains undeclared units

$$v_{12} = \mathrm{phi4a} \cdot [\mathrm{y5}] \tag{25}$$

7.13 Reaction R13

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

Reaction equation

$$\emptyset \xrightarrow{\mathrm{y1}} \mathrm{y6} \tag{26}$$

Modifier

Table 26: Properties of each modifier.

Id	Name	SBO
y1	E2F	

Product

Table 27: Properties of each product.

Id	Name	SBO
y6	AP-1	

Kinetic Law

Derived unit contains undeclared units

$$v_{13} = \mathrm{k6} \cdot [\mathrm{y1}] \tag{27}$$

7.14 Reaction R14

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

Reaction equation

$$\emptyset \longrightarrow \mathrm{y6} \tag{28}$$

Product

Table 28: Properties of each product.

Id	Name	SBO
y6	AP-1	

Kinetic Law

Derived unit not available

$$v_{14} = \mathrm{F6} \tag{29}$$

7.15 Reaction R15

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

Reaction equation

$$\mathrm{y6} \longrightarrow \emptyset \tag{30}$$

Reactant

Table 29: Properties of each reactant.

Id	Name	SBO
y6	AP-1	

Kinetic Law

Derived unit contains undeclared units

$$v_{15} = \mathrm{phi6} \cdot [\mathrm{y6}] \tag{31}$$

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.

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.

8.1 Species y1

Name E2F

Initial concentration $0.014\ \mathrm{mol} \cdot \mathrm{l}^{-1}$

This species takes part in five reactions (as a reactant in R2 and as a product in R1 and as a modifier in R3, R7, R13).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{y1} = v_1 - v_2 \tag{32}$$

8.2 Species y2

Name pRB

Initial concentration $0.0060\ \mathrm{mol} \cdot \mathrm{l}^{-1}$

This species takes part in four reactions (as a reactant in R4, R5 and as a product in R3 and as a modifier in R1).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{y2} = v_3 - v_4 - v_5 \tag{33}$$

8.3 Species y3

Name Phosphorylated pRB

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

This species takes part in two reactions (as a reactant in R6 and as a product in R4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{y3} = v_4 - v_6 \tag{34}$$

8.4 Species y4

Name inactive cycE_cdk2

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

This species takes part in five reactions (as a reactant in R9, R11 and as a product in R7, R8, R10).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{y4} = v_7 + v_8 + v_{10} - v_9 - v_{11} \tag{35}$$

8.5 Species y5

Name active cycE_cdk2

Initial concentration $10^{-4}\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in four reactions (as a reactant in R10, R12 and as a product in R9 and as a modifier in R4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{y5} = v_9 - v_{10} - v_{12} \tag{36}$$

8.6 Species y6

Name AP-1

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

This species takes part in four reactions (as a reactant in R15 and as a product in R13, R14 and as a modifier in R8).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{y6} = v_{13} + v_{14} - v_{15} \tag{37}$$

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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