SBML Model Report

Model name: "Obeyesekere1999_CellCycle"

May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 1 format. This model was created by Harish Dharuri[1] at March 16th 2008 at 7:31 p. m. and last time modified at May 27th 2014 at 10:24 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	7
events	0	constraints	0
reactions	10	function definitions	0
global parameters	21	unit definitions	0
rules	3	initial assignments	0

Model Notes

The model reproduces the time profiles of the different species depicted in Fig 3a of the paper. Model successfully reproduced using MathSBML.

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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 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
cell_1	cell		3	1	litre	☑	

3.1 Compartment cell_1

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

Name cell

4 Species

This model contains seven 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
D_1	D	cell_1	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
E_1	E	cell_1	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
RS_1	RS	cell_1	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
R_1	R	cell_1	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
X_1	X	cell_1	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
E2F_1	E2F	cell_1	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
RP_1	RP	cell_1	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟

5 Parameters

This model contains 21 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
aD_1	aD		0.400		☑
k_1	k		0.050		☑
GF_1	GF		6.300		☑
dD_1	dD		0.400		☑
aE_1	aE		0.160		☑
af_1	af		0.900		☑
theta_1	theta		1.500		☑
dE_1	dE		0.200		☑
pX_1	pX		0.480		☑
RT_1	RT		2.500		☑
pS_1	pS		0.600		☑
pD_1	pD		0.480		☑
qD_1	qD		0.600		☑
pE_1	pE		0.096		☑
qE_1	qE		0.600		☑
aX_1	aX		0.080		☑
f_1	f		0.200		☑
g_1	g		0.528		☑
dX_1	dX		1.040		☑
qX_1	qX		0.800		☑
unpho_RB			0.000		⊟

6 Rules

This is an overview of three rules.

6.1 Rule E2F_1

Rule E2F_1 is an assignment rule for species E2F_1:

$$\mathrm{E2F\_1} = \mathrm{theta\_1} - [\mathrm{RS\_1}] \tag{1}$$

6.2 Rule RP_1

Rule RP_1 is an assignment rule for species RP_1:

$$\mathrm{RP\_1} = \mathrm{RT\_1} - [\mathrm{RS\_1}] - [\mathrm{R\_1}] \tag{2}$$

6.3 Rule unpho_RB

Rule unpho_RB is an assignment rule for parameter unpho_RB:

$$\text{unpho\_RB} = [\text{R\_1}] + [\text{RS\_1}] \tag{3}$$

Derived unit $\text{mol} \cdot \text{l}^{-1}$

7 Reactions

This model contains ten 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	_1	cycD/CDK4 synthesis	$\emptyset \longrightarrow$ D_1	
2	cyclinCDK4degradation_1	cycD/CDK4 degradation	D_1 $\xrightarrow{\text{D_1, E_1}}$ $\emptyset$	
3	cyclin_1	cycE/CDK2 synthesis	$\emptyset \xrightarrow{\text{E2F_1}}$ E_1	
4	cycECDK2degradation_1	cycE/CDK2 degradation	E_1 $\xrightarrow{\text{E_1, X_1}}$ $\emptyset$	
5	pRBpdephosphorylation_1	pRBp dephosphorilation	$\emptyset \xrightarrow{\text{RP_1, X_1}}$ R_1	
6	pRBE2Fcomplexassociation_1	pRB/E2F complex association	R_1 $\xrightarrow{\text{RS_1, R_1, E2F_1}}$ RS_1	
7	pRBE2Fcomplexdeassociation_1	pRB/E2F complex deassociation via cycD/CDK4	RS_1 $\xrightarrow{\text{RS_1, D_1}}$ $\emptyset$	
8	_7	pRB/E2F complex deassociation via cycE/CDK2	RS_1 $\xrightarrow{\text{RS_1, E_1}}$ $\emptyset$	
9	cycleprogression_1	cycle progression	$\emptyset \xrightarrow{\text{E_1, E2F_1, X_1}}$ X_1	
10	cyclebreak_1	cycle break	X_1 $\xrightarrow{\text{X_1}}$ $\emptyset$	

7.1 Reaction _1

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

Name cycD/CDK4 synthesis

Reaction equation

$$\emptyset \longrightarrow \mathrm{D\_1} \tag{4}$$

Product

Table 6: Properties of each product.

Id	Name	SBO
D_1	D	

Kinetic Law

Derived unit not available

$$v_1 = \mathrm{aD\_1} \cdot \frac{\mathrm{k\_1} \cdot \mathrm{GF\_1}}{1 + \mathrm{k\_1} \cdot \mathrm{GF\_1}} \tag{5}$$

7.2 Reaction cyclinCDK4degradation_1

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

Name cycD/CDK4 degradation

Reaction equation

$$\mathrm{D\_1} \xrightarrow{\mathrm{D\_1,\ E\_1}} \emptyset \tag{6}$$

Reactant

Table 7: Properties of each reactant.

Id	Name	SBO
D_1	D	

Modifiers

Table 8: Properties of each modifier.

Id	Name	SBO
D_1	D	
E_1	E	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \mathrm{dD\_1} \cdot [\mathrm{E\_1}] \cdot [\mathrm{D\_1}] \tag{7}$$

7.3 Reaction cyclin_1

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

Name cycE/CDK2 synthesis

Reaction equation

$$\emptyset \xrightarrow{\mathrm{E2F\_1}} \mathrm{E\_1} \tag{8}$$

Modifier

Table 9: Properties of each modifier.

Id	Name	SBO
E2F_1	E2F	

Product

Table 10: Properties of each product.

Id	Name	SBO
E_1	E	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \mathrm{aE\_1} \cdot (1 + \mathrm{af\_1} \cdot [\mathrm{E2F\_1}]) \tag{9}$$

7.4 Reaction cycECDK2degradation_1

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

Name cycE/CDK2 degradation

Reaction equation

$$\mathrm{E\_1} \xrightarrow{\mathrm{E\_1,\ X\_1}} \emptyset \tag{10}$$

Reactant

Table 11: Properties of each reactant.

Id	Name	SBO
E_1	E	

Modifiers

Table 12: Properties of each modifier.

Id	Name	SBO
E_1	E	
X_1	X	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \mathrm{dE\_1} \cdot [\mathrm{X\_1}] \cdot [\mathrm{E\_1}] \tag{11}$$

7.5 Reaction pRBpdephosphorylation_1

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

Name pRB-p dephosphorilation

Reaction equation

$$\emptyset \xrightarrow{\mathrm{RP\_1,\ X\_1}} \mathrm{R\_1} \tag{12}$$

Modifiers

Table 13: Properties of each modifier.

Id	Name	SBO
RP_1	RP	
X_1	X	

Product

Table 14: Properties of each product.

Id	Name	SBO
R_1	R	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \frac{\mathrm{pX\_1} \cdot [\mathrm{RP\_1}] \cdot [\mathrm{X\_1}]}{\mathrm{qX\_1} + [\mathrm{RP\_1}] + [\mathrm{X\_1}]} \tag{13}$$

7.6 Reaction pRBE2Fcomplexassociation_1

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

Name pRB/E2F complex association

Reaction equation

$$\mathrm{R\_1} \xrightarrow{\mathrm{RS\_1,\ R\_1,\ E2F\_1}} \mathrm{RS\_1} \tag{14}$$

Reactant

Table 15: Properties of each reactant.

Id	Name	SBO
R_1	R	

Modifiers

Table 16: Properties of each modifier.

Id	Name	SBO
RS_1	RS	
R_1	R	
E2F_1	E2F	

Product

Table 17: Properties of each product.

Id	Name	SBO
RS_1	RS	

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \text{pS\_1} \cdot [\text{E2F\_1}] \cdot [\text{R\_1}] \tag{15}$$

7.7 Reaction pRBE2Fcomplexdeassociationviacyc DCDK4_1

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

Name pRB/E2F complex deassociation via cycD/CDK4

Reaction equation

$$\text{RS\_1} \xrightarrow{\text{RS\_1, D\_1}} \emptyset \tag{16}$$

Reactant

Table 18: Properties of each reactant.

Id	Name	SBO
RS_1	RS	

Modifiers

Table 19: Properties of each modifier.

Id	Name	SBO
RS_1	RS	
D_1	D	

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \frac{\mathrm{pD\_1} \cdot [\mathrm{RS\_1}] \cdot [\mathrm{D\_1}]}{\mathrm{qD\_1} + [\mathrm{RS\_1}] + [\mathrm{D\_1}]} \tag{17}$$

7.8 Reaction _7

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

Name pRB/E2F complex deassociation via cycE/CDK2

Reaction equation

$$\mathrm{RS\_1} \xrightarrow{\mathrm{RS\_1,\ E\_1}} \emptyset \tag{18}$$

Reactant

Table 20: Properties of each reactant.

Id	Name	SBO
RS_1	RS	

Modifiers

Table 21: Properties of each modifier.

Id	Name	SBO
RS_1	RS	
E_1	E	

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \frac{\mathrm{pE\_1} \cdot [\mathrm{RS\_1}] \cdot [\mathrm{E\_1}]}{\mathrm{qE\_1} + [\mathrm{RS\_1}] + [\mathrm{E\_1}]} \tag{19}$$

7.9 Reaction `cycleprogression_1`

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

Name cycle progression

Reaction equation

$$\emptyset \xrightarrow{\mathrm{E\_1,\ E2F\_1,\ X\_1}} \mathrm{X\_1} \tag{20}$$

Modifiers

Table 22: Properties of each modifier.

Id	Name	SBO
`E_1`	E	
`E2F_1`	E2F	
`X_1`	X	

Product

Table 23: Properties of each product.

Id	Name	SBO
`X_1`	X	

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \mathrm{aX\_1} \cdot [\mathrm{E\_1}] + \mathrm{f\_1} \cdot [\mathrm{E2F\_1}] + \mathrm{g\_1} \cdot [\mathrm{X\_1}]^2 \cdot [\mathrm{E\_1}] \tag{21}$$

7.10 Reaction `cyclebreak_1`

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

Name cycle break

Reaction equation

$$\mathrm{X\_1} \xrightarrow{\mathrm{X\_1}} \emptyset \tag{22}$$

Reactant

Table 24: Properties of each reactant.

Id	Name	SBO
X_1	X	

Modifier

Table 25: Properties of each modifier.

Id	Name	SBO
X_1	X	

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = \mathrm{dX\_1} \cdot [\mathrm{X\_1}] \tag{23}$$

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 D_1

Name D

Initial amount 0.1 mol

This species takes part in four reactions (as a reactant in cyclinCDK4degradation_1 and as a product in _1 and as a modifier in cyclinCDK4degradation_1, pRBE2Fcomplexdeassociationviacyc DCDK4-_1).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{D\_1} = v_1 - v_2 \tag{24}$$

8.2 Species E_1

Name E

Initial amount 0.6 mol

This species takes part in six reactions (as a reactant in cycECDK2degradation_1 and as a product in cyclin_1 and as a modifier in cyclinCDK4degradation_1, cycECDK2degradation_1, _7, cycleprogression_1).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{E\_1} = v_3 - v_4 \tag{25}$$

8.3 Species RS_1

Name RS

Initial amount 1 mol

This species takes part in six reactions (as a reactant in pRBE2Fcomplexdeassociationviacyc DCDK4-_1, _7 and as a product in pRBE2Fcomplexassociation_1 and as a modifier in pRBE2Fcomplexassociation-_1, pRBE2Fcomplexdeassociationviacyc DCDK4_1, _7).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{RS\_1} = v_6 - v_7 - v_8 \tag{26}$$

8.4 Species R_1

Name R

Initial amount 0.5 mol

This species takes part in three reactions (as a reactant in pRBE2Fcomplexassociation_1 and as a product in pRBpdephosphorylation_1 and as a modifier in pRBE2Fcomplexassociation-_1).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{R\_1} = v_5 - v_6 \tag{27}$$

8.5 Species X_1

Name X

Initial amount 0.7 mol

This species takes part in six reactions (as a reactant in cyclebreak_1 and as a product in cycleprogression_1 and as a modifier in cycECDK2degradation_1, pRBpdephosphorylation-_1, cycleprogression_1, cyclebreak_1).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{X\_1} = v_9 - v_{10} \tag{28}$$

8.6 Species E2F_1

Name E2F

Involved in rule E2F_1

This species takes part in three reactions (as a modifier in cyclin_1, pRBE2Fcomplexassociation_1, cycleprogression_1) and is also involved in one rule which determines this species' quantity.

8.7 Species RP_1

Name RP

Involved in rule RP_1

This species takes part in one reaction (as a modifier in pRBpdephosphorylation_1) 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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