SBML Model Report

Model name: “Srividhya2006_CellCycle”

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1 General Overview

This is a document in SBML Level 2 Version 1 format. This model was created by the following four authors: Harish Dharuri[1], Lukas Endler[2], Vijayalakshmi Chelliah[3] and Srividhya Jeyaram[4] at October thirteenth 2008 at 12:53 a. m. and last time modified at April eighth 2016 at 3:47 p. m. Table 1 shows 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	11
events	1	constraints	0
reactions	13	function definitions	3
global parameters	35	unit definitions	0
rules	4	initial assignments	0

Model Notes

In this model the values of „free CDK„ (Id: x2), „cdc25_P„ (x4) „Wee1_P„ (Id: y5) and „APC„ (Id: y6) are assigned using the parameters describing the total concentrations totcdk (Id: c)), totcdc5, totwee1 and totAPC. So if you want to change the levels of these proteins, you need to change the values ofthese parameters.

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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`	cell		3	1	litre	☑	

3.1 Compartment `cell`

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

Name cell

4 Species

This model contains eleven species. The boundary condition of four of these species is set to `true` so that these species' amount cannot be changed by any reaction. Section 10 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
x1	cyclin	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☐
x2	free CDK	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☑
x3	MPF	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☐
x4	cdc25_P	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☑
x5	Wee1	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☐
x6	APC_P	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☐
m	cell_mass	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☐
y4	cdc25	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☐
y5	Wee1_P	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☑
y6	APC	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☑
Pre_MPF	Pre_MPF	cell	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	☐	☐

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5 Parameters

This model contains 35 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
vf	vf		0.215		☑
kf	kf		1.000		☑
kc	kc		0.050		☑
Bc	Bc		3.500		☑
kd	kd		0.200		☑
B2	B2		3.300		☑
vM1	vM1		0.700		☑
a1	a1		1.200		☑
Ka	Ka		0.500		☑
j1	j1		0.010		☑
B1	B1		5.000		☑
vM1_2	v'M1		0.550		☑
j1_2	j'1		0.010		☑
vM2	vM2		0.410		☑
a2	a2		1.000		☑
j2	j2		0.010		☑
vM2_2	v'M2		1.000		☑
j3	j'3		0.010		☑
j2_2	j'2		0.010		☑
vM3	vM3		1.000		☑
j3_2	j3		0.010		☑
vM3_2	v'M3		1.000		☑
B3	B3		1.000		☑
vM4	vM4		0.700		☑
a4	a4		2.000		☑
tau	tau		5.000		☑
j4	j4		0.010		☑
vM4_2	v'M4		1.000		☑
j4_2	j'4		0.010		☑
mu	mu		0.010		☑
a	a		10.000		☑
totcdc25	totcdc25		1.000		☑
totwee1	totwee1		1.000		☑
totAPC	totAPC		1.000		☑
c	totcdk		1.100		☑

6 Function definitions

This is an overview of three function definitions.

6.1 Function definition Mass_Action_0

Name Mass_Action_0

Argument k1

Mathematical Expression

$$\mathrm{k1} \tag{1}$$

6.2 Function definition Mass_Action_2

Name Mass_Action_2

Arguments k1, S1, S2

Mathematical Expression

$$\mathrm{k1} \cdot \mathrm{S1} \cdot \mathrm{S2} \tag{2}$$

6.3 Function definition Mass_Action_1

Name Mass_Action_1

Arguments k1, S1

Mathematical Expression

$$\mathrm{k1} \cdot \mathrm{S1} \tag{3}$$

7 Rules

This is an overview of four rules.

7.1 Rule x4

Rule x4 is an assignment rule for species x4:

$$\mathrm{x4} = \mathrm{totcdc25} - [\mathrm{y4}] \tag{4}$$

7.2 Rule y5

Rule y5 is an assignment rule for species y5:

$$\mathrm{y5} = \mathrm{totwee1} - [\mathrm{x5}] \tag{5}$$

7.3 Rule y6

Rule y6 is an assignment rule for species y6:

$$\mathrm{y6} = \mathrm{totAPC} - [\mathrm{x6}] \tag{6}$$

7.4 Rule x2

Rule x2 is an assignment rule for species x2:

$$\mathrm{x2} = \mathrm{c} - [\mathrm{Pre\_MPF}] - [\mathrm{x3}] \tag{7}$$

8 Event

This is an overview of one event. Each event is initiated whenever its trigger condition switches from `false` to `true`. A delay function postpones the effects of an event to a later time point. At the time of execution, an event can assign values to species, parameters or compartments if these are not set to constant.

8.1 Event event_0

Name cell_division

Trigger condition

$$[\mathrm{x3}] < 0.2 \tag{8}$$

Assignment

$$\mathrm{m} = \frac{[\mathrm{m}]}{2} \tag{9}$$

9 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	cyclinsynthesis	cyclin synthesis	$\emptyset \longrightarrow x1$	
2	cyclincdkcomplexformation	cyclin/cdk complex formation	$x1 + x2 \longrightarrow Pre\_MPF$	
3	cyclindegradation	cyclin degradation	$x1 \xrightarrow{x6} \emptyset$	
4	MPFdissociation	MPF cyclin subunit degradation	$x3 \xrightarrow{x6} x2$	
5	PreMPFMPFtransition	Pre-MPF -> MPF transition	$Pre\_MPF \xrightarrow{x4} x3$	
6	MPFPreMPFtransition	MPF -> Pre-MPF transition	$x3 \xrightarrow{x5} Pre\_MPF$	
7	cdc25phosphorylation	cdc25 phosphorylation	$y4 \xrightarrow{m,\ x3} x4$	
8	cdc25dephosphorylation	cdc25 dephosphorylation	$x4 \longrightarrow y4$	
9	wee1dephosphorylation	wee1 dephosphorylation	$y5 \longrightarrow x5$	
10	wee1phosphorylation	wee1 phosphorylation	$x5 \xrightarrow{x3,\ m} y5$	
11	_2	APC phosphorylation	$y6 \xrightarrow{m,\ x3} x6$	
12	APCdephosphorylation	APC dephosphorylation	$x6 \longrightarrow y6$	
13	cellmass	cell growth	$\emptyset \longrightarrow m$	

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9.1 Reaction `cyclinsythesis`

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

Name cyclin synthesis

Reaction equation

$$\emptyset \longrightarrow \mathrm{x1} \tag{10}$$

Product

Table 6: Properties of each product.

Id	Name	SBO
x1	cyclin	

Kinetic Law

Derived unit not available

$$v_1 = \mathrm{Mass\_Action\_0}\,(\mathrm{vf}) \tag{11}$$

$$\mathrm{Mass\_Action\_0}\,(\mathrm{k1}) = \mathrm{k1} \tag{12}$$

9.2 Reaction `cyclincdkcomplexformation`

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

Name cyclin/cdk complex formation

Reaction equation

$$\mathrm{x1} + \mathrm{x2} \longrightarrow \mathrm{Pre\_MPF} \tag{13}$$

Reactants

Table 7: Properties of each reactant.

Id	Name	SBO
x1	cyclin	
x2	free CDK	

Product

Table 8: Properties of each product.

Id	Name	SBO
`Pre_MPF`	Pre_MPF	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \text{Mass\_Action\_2}\,(\text{kf}, [\text{x1}], [\text{x2}]) \tag{14}$$

$$\text{Mass\_Action\_2}\,(\text{k1}, \text{S1}, \text{S2}) = \text{k1} \cdot \text{S1} \cdot \text{S2} \tag{15}$$

9.3 Reaction `cyclindegradation`

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

Name cyclin degradation

Reaction equation

$$\text{x1} \xrightarrow{\text{x6}} \emptyset \tag{16}$$

Reactant

Table 9: Properties of each reactant.

Id	Name	SBO
`x1`	cyclin	

Modifier

Table 10: Properties of each modifier.

Id	Name	SBO
`x6`	APC_P	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = [\mathrm{x1}] \cdot (\mathrm{kc} + \mathrm{Bc} \cdot [\mathrm{x6}]) \tag{17}$$

9.4 Reaction `MPFdissociation`

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

Name MPF cyclin subunit degradation

Reaction equation

$$\mathrm{x3} \xrightarrow{\mathrm{x6}} \mathrm{x2} \tag{18}$$

Reactant

Table 11: Properties of each reactant.

Id	Name	SBO
x3	MPF	

Modifier

Table 12: Properties of each modifier.

Id	Name	SBO
x6	APC_P	

Product

Table 13: Properties of each product.

Id	Name	SBO
x2	free CDK	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \mathrm{kd} \cdot (1 + \mathrm{B2} \cdot [\mathrm{x6}]) \cdot [\mathrm{x3}] \tag{19}$$

9.5 Reaction PreMPFMPFtransition

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

Name Pre-MPF -> MPF transition

Reaction equation

$$\text{Pre\_MPF} \xrightarrow{\text{x4}} \text{x3} \tag{20}$$

Reactant

Table 14: Properties of each reactant.

Id	Name	SBO
Pre_MPF	Pre_MPF	

Modifier

Table 15: Properties of each modifier.

Id	Name	SBO
x4	cdc25_P	

Product

Table 16: Properties of each product.

Id	Name	SBO
x3	MPF	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \text{vM1} \cdot \left(1 + \frac{\text{a1} \cdot [\text{x4}]}{\text{Ka} + [\text{x4}]}\right) \cdot \frac{[\text{Pre\_MPF}]}{\text{j1} + [\text{Pre\_MPF}]} \tag{21}$$

9.6 Reaction MPFPreMPFtransition

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

Name MPF -> Pre-MPF transition

Reaction equation

$$\mathrm{x3} \xrightarrow{\mathrm{x5}} \mathrm{Pre\_MPF} \tag{22}$$

Reactant

Table 17: Properties of each reactant.

Id	Name	SBO
x3	MPF	

Modifier

Table 18: Properties of each modifier.

Id	Name	SBO
x5	Wee1	

Product

Table 19: Properties of each product.

Id	Name	SBO
Pre_MPF	Pre_MPF	

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \mathrm{vM1\_2} \cdot \left(1 + \frac{\mathrm{B1} \cdot [\mathrm{x5}]}{\mathrm{Ka} + [\mathrm{x5}]}\right) \cdot \frac{[\mathrm{x3}]}{\mathrm{j1\_2} + [\mathrm{x3}]} \tag{23}$$

9.7 Reaction cdc25phosphorylation

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

Name cdc25 phosphorylation

Reaction equation

$$\mathrm{y4} \xrightarrow{\mathrm{m,\ x3}} \mathrm{x4} \tag{24}$$

Reactant

Table 20: Properties of each reactant.

Id	Name	SBO
y4	cdc25	

Modifiers

Table 21: Properties of each modifier.

Id	Name	SBO
m	cell_mass	
x3	MPF	

Product

Table 22: Properties of each product.

Id	Name	SBO
x4	cdc25_P	

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \mathrm{vM2} \cdot \left(1 + \frac{\mathrm{a2} \cdot [\mathrm{m}] \cdot [\mathrm{x3}]}{\mathrm{Ka} + [\mathrm{m}] \cdot [\mathrm{x3}]}\right) \cdot \frac{1 - [\mathrm{x4}]}{\mathrm{j2} + 1 - [\mathrm{x4}]} \tag{25}$$

9.8 Reaction cdc25dephosphorylation

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

Name cdc25 dephosphorylation

Reaction equation

$$\mathrm{x4} \longrightarrow \mathrm{y4} \tag{26}$$

Reactant

Table 23: Properties of each reactant.

Id	Name	SBO
x4	cdc25_P	

Product

Table 24: Properties of each product.

Id	Name	SBO
y4	cdc25	

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \frac{\mathrm{vM2\_2} \cdot [\mathrm{x4}]}{\mathrm{j2\_2} + [\mathrm{x4}]} \tag{27}$$

9.9 Reaction `wee1dephosphorylation`

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

Name wee1 dephosphorylation

Reaction equation

$$\mathrm{y5} \longrightarrow \mathrm{x5} \tag{28}$$

Reactant

Table 25: Properties of each reactant.

Id	Name	SBO
y5	Wee1_P	

Product

Table 26: Properties of each product.

Id	Name	SBO
x5	Wee1	

Id	Name	SBO

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \mathrm{vM3} \cdot \frac{1 - [\mathrm{x5}]}{\mathrm{j3\_2} + 1 - [\mathrm{x5}]} \tag{29}$$

9.10 Reaction `wee1phosphorylation`

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

Name wee1 phosphorylation

Reaction equation

$$\mathrm{x5} \xrightarrow{\mathrm{x3,\ m}} \mathrm{y5} \tag{30}$$

Reactant

Table 27: Properties of each reactant.

Id	Name	SBO
`x5`	Wee1	

Modifiers

Table 28: Properties of each modifier.

Id	Name	SBO
`x3`	MPF	
`m`	cell_mass	

Product

Table 29: Properties of each product.

Id	Name	SBO
`y5`	Wee1_P	

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = \text{vM3\_2} \cdot \left(1 + \frac{\text{B3} \cdot [\text{m}] \cdot [\text{x3}]}{\text{Ka} + [\text{m}] \cdot [\text{x3}]}\right) \cdot \frac{[\text{x5}]}{\text{j3} + [\text{x5}]} \tag{31}$$

9.11 Reaction _2

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

Name APC phosphorylation

Reaction equation

$$\text{y6} \xrightarrow{\text{m, x3}} \text{x6} \tag{32}$$

Reactant

Table 30: Properties of each reactant.

Id	Name	SBO
y6	APC	

Modifiers

Table 31: Properties of each modifier.

Id	Name	SBO
m	cell_mass	
x3	MPF	

Product

Table 32: Properties of each product.

Id	Name	SBO
x6	APC_P	

Kinetic Law

Derived unit contains undeclared units

$$v_{11} = \mathrm{vM4} \cdot \frac{\left(1 + \frac{\mathrm{a4} \cdot [\mathrm{m}] \cdot \mathrm{delay}}{\mathrm{Ka} + [\mathrm{m}] \cdot \mathrm{delay}}\right) \cdot (1 - [\mathrm{x6}])}{\mathrm{j4} + (1 - [\mathrm{x6}])} \tag{33}$$

9.12 Reaction `APCdephosphorylation`

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

Name APC dephosphorylation

Reaction equation

$$\mathrm{x6} \longrightarrow \mathrm{y6} \tag{34}$$

Reactant

Table 33: Properties of each reactant.

Id	Name	SBO
`x6`	APC_P	

Product

Table 34: Properties of each product.

Id	Name	SBO
`y6`	APC	

Kinetic Law

Derived unit contains undeclared units

$$v_{12} = \frac{\mathrm{vM4\_2} \cdot [\mathrm{x6}]}{\mathrm{j4\_2} + [\mathrm{x6}]} \tag{35}$$

9.13 Reaction `cellmass`

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

Name cell growth

Reaction equation

$$\emptyset \longrightarrow \mathrm{m} \tag{36}$$

Product

Table 35: Properties of each product.

Id	Name	SBO
m	cell_mass	

Kinetic Law

Derived unit contains undeclared units

$$v_{13} = \mathrm{mu} \cdot [\mathrm{m}] \cdot \left(1 - \frac{[\mathrm{m}]}{\mathrm{a}}\right) \tag{37}$$

10 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.

10.1 Species x1

Name cyclin

Initial amount 0.01 mol

This species takes part in three reactions (as a reactant in `cyclincdkcomplexformation`, `cyclindegradation` and as a product in `cyclinsythesis`).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{x1} = v_1 - v_2 - v_3 \tag{38}$$

10.2 Species x2

Name free CDK

Involved in rule x2

This species takes part in two reactions (as a reactant in `cyclincdkcomplexformation` and as a product in `MPFdissociation`). Not these but one rule determines the species' quantity because this species is on the boundary of the reaction system.

10.3 Species x3

Name MPF

Initial amount 0.1 mol

This species takes part in six reactions (as a reactant in MPFdissociation, MPFPreMPFtransition and as a product in PreMPFMPFtransition and as a modifier in cdc25phosphorylation, wee1phosphorylation, _2).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{x3} = v_5 - v_4 - v_6 \tag{39}$$

10.4 Species x4

Name cdc25_P

Involved in rule x4

This species takes part in three reactions (as a reactant in cdc25dephosphorylation and as a product in cdc25phosphorylation and as a modifier in PreMPFMPFtransition). Not these but one rule determines the species' quantity because this species is on the boundary of the reaction system.

10.5 Species x5

Name Wee1

Initial amount 0.1 mol

This species takes part in three reactions (as a reactant in wee1phosphorylation and as a product in wee1dephosphorylation and as a modifier in MPFPreMPFtransition).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{x5} = v_9 - v_{10} \tag{40}$$

10.6 Species x6

Name APC_P

Initial amount 0.1 mol

This species takes part in four reactions (as a reactant in APCdephosphorylation and as a product in _2 and as a modifier in cyclindegradation, MPFdissociation).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{x6} = v_{11} - v_{12} \tag{41}$$

10.7 Species m

Name cell_mass

Initial amount 0.473 mol

Involved in event event_0

This species takes part in four reactions (as a product in cellmass and as a modifier in cdc25phosphorylation, wee1phosphorylation, _2).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{m} = v_{13} \tag{42}$$

Furthermore, one event influences this species' rate of change.

10.8 Species y4

Name cdc25

Initial amount 0.9 mol

This species takes part in two reactions (as a reactant in cdc25phosphorylation and as a product in cdc25dephosphorylation).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{y4} = v_8 - v_7 \tag{43}$$

10.9 Species y5

Name Wee1_P

Involved in rule y5

This species takes part in two reactions (as a reactant in wee1dephosphorylation and as a product in wee1phosphorylation). Not these but one rule determines the species' quantity because this species is on the boundary of the reaction system.

10.10 Species y6

Name APC

Involved in rule y6

This species takes part in two reactions (as a reactant in _2 and as a product in APCdephosphorylation). Not these but one rule determines the species' quantity because this species is on the boundary of the reaction system.

10.11 Species Pre_MPF

Name Pre_MPF

Initial amount 0.2 mol

This species takes part in three reactions (as a reactant in PreMPFMPFtransition and as a product in cyclincdkcomplexformation, MPFPreMPFtransition).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Pre\_MPF} = v_2 + v_6 - v_5 \tag{44}$$

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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