SBML Model Report

Model name: “Ciliberto2003 - CyclinE / Cdk2 timer in the cell cycle of Xenopus laevis embryo”

May 17, 2018

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by the following two authors: Rahuman Sheriff[1] and Matthieu MAIRE[2] at April 23rd 2018 at 9:03 a. m. and last time modified at May first 2018 at 12:26 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	16
events	0	constraints	0
reactions	30	function definitions	13
global parameters	25	unit definitions	5
rules	6	initial assignments	0

Model Notes

Ciliberto2003 - CyclinE / Cdk2 timer in thecell cycle of Xenopus laevis embryo

[1]EMBL-EBI, sheriff@ebi.ac.uk
[2]EMBL-EBI, matt.maire@free.fr

This model is described in the article:A kinetic model of the cyclin E/Cdk2 developmental timer in Xenopus laevis embryos.Ciliberto A, Petrus MJ, Tyson JJ, Sible JC.Biophys. Chem. 2003 Jul; 104(3): 573-589

Abstract:

Early cell cycles of Xenopus laevis embryos are characterized by rapid oscillations in the activity of two cyclin-dependent kinases. Cdk1 activity peaks at mitosis, driven by periodic degradation of cyclins A and B. In contrast, Cdk2 activity oscillates twice per cell cycle, despite a constant level of its partner, cyclin E. Cyclin E degrades at a fixed time after fertilization, normally corresponding to the midblastula transition. Based on published data and new experiments, we constructed a mathematical model in which: (1) oscillations in Cdk2 activity depend upon changes in phosphorylation, (2) Cdk2 participates in a negative feedback loop with the inhibitory kinase Wee1; (3) cyclin E is cooperatively removed from the oscillatory system; and (4) removed cyclin E is degraded by a pathway activated by cyclin E/Cdk2 itself. The model's predictions about embryos injected with Xic1, a stoichiometric inhibitor of cyclin E/Cdk2, were experimentally validated.

This model is hosted on BioModels Database and identified by: BIOMD0000000697.

To cite BioModels Database, please use: Chelliah V et al. BioModels: ten-year anniversary. Nucl. Acids Res. 2015, 43(Database issue):D542-8.

2 Unit Definitions

This is an overview of seven unit definitions of which two are predefined by SBML and not mentioned in the model.

2.1 Unit `volume`

Name volume

Definition ml

2.2 Unit `time`

Name time

Definition 60 s

2.3 Unit `substance`

Name substance

Definition mmol

2.4 Unit unit_0

Name 1

Definition dimensionless^{0}

2.5 Unit unit_1

Name 1/s

Definition s^{-1}

2.6 Unit area

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

Definition m^{2}

2.7 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	embryo		3	1	litre	☑	

3.1 Compartment compartment

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

Name embryo

4 Species

This model contains 16 species. The boundary condition of three of these species is set to `true` so that these species' amount cannot be changed by any reaction. Section 9 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
PCdk2_CycE	PCdk2_CycE	compartment	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	☐	☐
Cdk2_CycE	Cdk2_CycE	compartment	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	☐	☐
Wee1_a	Wee1_a	compartment	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	☐	☐
Wee1_total	Wee1_total	compartment	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	☑	☑
Cdk2_CycErem	Cdk2_CycErem	compartment	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	☐	☐
PCdk2_CycErem	PCdk2_CycErem	compartment	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	☐	☐
Deg_a	Deg_CycE	compartment	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	☐	☐
Xic	Xic	compartment	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	☐	☐
Xic_Cdk2_CycE	Xic_Cdk2_CycE	compartment	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	☐	☐
Xic_PCdk2_CycE	Xic_PCdk2_CycE	compartment	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	☐	☐
Xic_Cdk2_CycErem	Xic_Cdk2_CycErem	compartment	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	☐	☐
Xic_PCdk2_CycErem	Xic_PCdk2_CycErem	compartment	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	☐	☐
Xicrem	Xicrem	compartment	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	☐	☐
Cyc_total	Cyc_total	compartment	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	☐	☑
Xic_total	Xic_total	compartment	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	☐	☑
Kin_a	Kin_a	compartment	$\mathrm{mmol} \cdot \mathrm{ml}^{-1}$	☐	☐

5 Parameters

This model contains 25 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Jwact	Jwact		0.010		☑
Jwinact	Jwinact		0.010	dimensionless^0	☑
kwact	kwact		0.750	s^{-1}	☑
kwinact	kwinact		1.500	s^{-1}	☑
Jiact	Jiact		0.010		☑
Jiinact	Jiinact		0.010		☑
kiact	kiact		0.150	s^{-1}	☑
kiinact	kiinact		0.600	s^{-1}	☑
Heav	Heav		0.000	dimensionless^0	⊟
kdact	kdact		0.023	s^{-1}	☑
theta	theta		0.300		☑
kwee	kwee		1.500	s^{-1}	☑
k25A	k25A		0.100	s^{-1}	☑
kon	kon		0.020	s^{-1}	☑
koff	koff		10^{-4}	s^{-1}	☑
kassoc	kassoc		0.100	s^{-1}	☑
kdissoc	kdissoc		0.001	s^{-1}	☑
kedeg	kedeg		0.017	s^{-1}	☑
kxdeg	kxdeg		0.010	s^{-1}	☑
phi	phi		0.039	dimensionless^0	⊟
epsilon	epsilon		0.001		☑
pool	pool		0.000	dimensionless^0	⊟
n	n		4.000		☑
L	L		0.400		☑
x	x		−0.300		⊟

6 Function definitions

This is an overview of 13 function definitions.

6.1 Function definition function_removed_from_oscillatory_system_1

Name function removed from oscillatory system_1

Arguments [Cdk2_CycE], kon, phi

Mathematical Expression

$$\text{kon} \cdot \text{phi} \cdot [\text{Cdk2\_CycE}] \tag{1}$$

6.2 Function definition function_removed_from_oscillatory_system_2

Name function removed from oscillatory system_2

Arguments [PCdk2_CycE], kon, phi

Mathematical Expression

$$\text{kon} \cdot \text{phi} \cdot [\text{PCdk2\_CycE}] \tag{2}$$

6.3 Function definition Function_for_degradation_of_Xic_Cyc_Cdk_1

Name Function for degradation of Xic_Cyc_Cdk_1

Arguments [Deg_a], [Xic_PCdk2_CycErem], kedeg

Mathematical Expression

$$\text{kedeg} \cdot [\text{Xic\_PCdk2\_CycErem}] \cdot [\text{Deg\_a}] \tag{3}$$

6.4 Function definition Function_for_degradation_of_Xic_Cyc_Cdk_2

Name Function for degradation of Xic_Cyc_Cdk_2

Arguments [Deg_a], [Xic_Cdk2_CycErem], kedeg

Mathematical Expression

$$\text{kedeg} \cdot [\text{Xic\_Cdk2\_CycErem}] \cdot [\text{Deg\_a}] \tag{4}$$

6.5 Function definition function_Hill_Cdk2_CycE_removal_1

Name function Hill_Cdk2_CycE_removal_1

Arguments Heav, kdact

Mathematical Expression

$$\text{kdact} \cdot \text{Heav} \tag{5}$$

6.6 Function definition Function_phosphorylation_with_Wee1_1

Name Function phosphorylation with Wee1_1

Arguments [Wee1_a], [Xic_Cdk2_CycE], kwee

Mathematical Expression

$$\text{kwee} \cdot [\text{Wee1\_a}] \cdot [\text{Xic\_Cdk2\_CycE}] \tag{6}$$

6.7 Function definition Function_phosphorylation_with_Wee1_2

Name Function phosphorylation with Wee1_2

Arguments [Cdk2_CycE], [Wee1_a], kwee

Mathematical Expression

$$\text{kwee} \cdot [\text{Wee1\_a}] \cdot [\text{Cdk2\_CycE}] \tag{7}$$

6.8 Function definition Function_for_Kin_a_1

Name Function for Kin_a_1

Arguments [Cdk2_CycE], Jiact, Jiinact, [Kin_a], kiact, kiinact

Mathematical Expression

$$\frac{\text{kiact} \cdot (1 - [\text{Kin\_a}])}{\text{Jiact} + 1 - [\text{Kin\_a}]} - \frac{\text{kiinact} \cdot [\text{Cdk2\_CycE}] \cdot [\text{Kin\_a}]}{\text{Jiinact} + [\text{Kin\_a}]} \tag{8}$$

6.9 Function definition Function_for_degradation_of_Xic_Cyc_Cdk_3

Name Function for degradation of Xic_Cyc_Cdk_3

Arguments [Cdk2_CycErem], [Deg_a], kedeg

Mathematical Expression

$$\text{kedeg} \cdot [\text{Cdk2\_CycErem}] \cdot [\text{Deg\_a}] \tag{9}$$

6.10 Function definition Function_for_degradation_of_Xic_Cyc_Cdk_4

Name Function for degradation of Xic_Cyc_Cdk_4

Arguments [Deg_a], [PCdk2_CycErem], kedeg

Mathematical Expression

$$\text{kedeg} \cdot [\text{PCdk2\_CycErem}] \cdot [\text{Deg\_a}] \tag{10}$$

6.11 Function definition function_removed_from_oscillatory_system_3

Name function removed from oscillatory system_3

Arguments [Xic_PCdk2_CycE], kon, phi

Mathematical Expression

$$\text{kon} \cdot \text{phi} \cdot [\text{Xic\_PCdk2\_CycE}] \tag{11}$$

6.12 Function definition function_removed_from_oscillatory_system_4

Name function removed from oscillatory system_4

Arguments [Xic_Cdk2_CycE], kon, phi

Mathematical Expression

$$\text{kon} \cdot \text{phi} \cdot [\text{Xic\_Cdk2\_CycE}] \tag{12}$$

6.13 Function definition Function_for_Wee1_a_1

Name Function for Wee1_a_1

Arguments Jwact, Jwinact, [Kin_a], [Wee1_a], [Wee1_total], kwact, kwinact

Mathematical Expression

$$\frac{\text{kwact} \cdot ([\text{Wee1\_total}] - [\text{Wee1\_a}])}{\text{Jwact} + [\text{Wee1\_total}] - [\text{Wee1\_a}]} - \frac{\text{kwinact} \cdot [\text{Kin\_a}] \cdot [\text{Wee1\_a}]}{\text{Jwinact} + [\text{Wee1\_a}]} \tag{13}$$

7 Rules

This is an overview of six rules.

7.1 Rule Cyc_total

Rule Cyc_total is an assignment rule for species Cyc_total:

$$\begin{aligned}\text{Cyc\_total} = {} & [\text{Xic\_PCdk2\_CycE}] + [\text{Xic\_Cdk2\_CycE}] + [\text{Xic\_PCdk2\_CycErem}] \\ & + [\text{Xic\_Cdk2\_CycErem}] + [\text{PCdk2\_CycErem}] \\ & + [\text{Cdk2\_CycErem}] + [\text{Cdk2\_CycE}] + [\text{PCdk2\_CycE}]\end{aligned} \tag{14}$$

Derived unit $\text{mmol} \cdot \text{ml}^{-1}$

7.2 Rule Xic_total

Rule Xic_total is an assignment rule for species Xic_total:

$$\text{Xic\_total} = \frac{[\text{Xic}] + [\text{Xic\_PCdk2\_CycE}] + [\text{Xic\_Cdk2\_CycE}] + [\text{Xic\_PCdk2\_CycErem}] + [\text{Xic\_Cdk2\_CycErem}] + [\text{Xicrem}]}{3} \tag{15}$$

7.3 Rule pool

Rule pool is an assignment rule for parameter pool:

$$\text{pool} = [\text{Cdk2\_CycErem}] + [\text{PCdk2\_CycErem}] + [\text{Xic\_Cdk2\_CycErem}] + [\text{Xic\_PCdk2\_CycErem}] \tag{16}$$

Derived unit $\text{mmol} \cdot \text{ml}^{-1}$

7.4 Rule `phi`

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

$$\text{phi} = \frac{\text{epsilon} + \text{pool}^{\text{n}}}{\text{L}^{\text{n}} + \text{pool}^{\text{n}}} \tag{17}$$

7.5 Rule `x`

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

$$\text{x} = [\text{Cdk2\_CycErem}] - \text{theta} \tag{18}$$

7.6 Rule `Heav`

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

$$\text{Heav} = \begin{cases} 0 & \text{if x} < 0 \\ 1 & \text{otherwise} \end{cases} \tag{19}$$

8 Reactions

This model contains 30 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	Xic_Cdk2_CycE_association	Xic_Cdk2_CycE_association	Xic + Cdk2_CycE ⟶ Xic_Cdk2_CycE	
2	Xic_Cdk2_CycErem_association	Xic_Cdk2_CycErem_association	Xic + Cdk2_CycErem ⟶ Xic_Cdk2_CycErem	
3	Xic_Cdk2_CycE_dissociation	Xic_Cdk2_CycE_dissociation	Xic_Cdk2_CycE ⟶ Xic + Cdk2_CycE	
4	Xic_Cdk2_CycErem_dissociation	Xic_Cdk2_CycErem_dissociation	Xic_Cdk2_CycErem ⟶ Xic + Cdk2_CycErem	
5	Cdk2_CycErem_to_not_rem	Cdk2_CycErem_to_not_rem	Cdk2_CycErem ⟶ Cdk2_CycE	
6	PCdk2_CycE_to_not_rem	PCdk2_CycE_to_not_rem	PCdk2_CycErem ⟶ PCdk2_CycE	
7	Cdk2_CycE_to_rem	Cdk2_CycE_to_rem	Cdk2_CycE ⟶ Cdk2_CycErem	
8	PCdk2_CycE_to_rem	PCdk2_CycE_to_rem	PCdk2_CycE ⟶ PCdk2_CycErem	
9	X_degadation	X_degadation	Xic_Cdk2_CycErem ⟶ Cdk2_CycErem	
10	X_degradation_phosphorylated_complex	X_degradation_phosphorylated_complex	Xic_PCdk2_CycErem ⟶ PCdk2_CycErem	

№	Id	Name	Reaction Equation	SBO
11	Degradation_XicPCdk2_CycErem	Degradation_XicPCdk2_CycErem	$\text{Xic\_PCdk2\_CycErem} \xrightarrow{\text{Deg\_a}} \text{Xicrem}$	
12	Degradation_XicCdk2_CycErem	Degradation_XicCdk2_CycErem	$\text{Xic\_Cdk2\_CycErem} \xrightarrow{\text{Deg\_a}} \text{Xicrem}$	
13	Dephos_Xic_PCdk2_CycE	Dephos_Xic_PCdk2_CycE	$\text{Xic\_PCdk2\_CycE} \longrightarrow \text{Xic\_Cdk2\_CycE}$	
14	Dephos_PCdk2_CycE	Dephos_PCdk2_CycE	$\text{PCdk2\_CycE} \longrightarrow \text{Cdk2\_CycE}$	
15	Degradation_increase	Degradation_increase	$\emptyset \longrightarrow \text{Deg\_a}$	
16	Phos_Xic_PCdk2_CycE	Phos_Xic_PCdk2_CycE	$\text{Xic\_Cdk2\_CycE} \xrightarrow{\text{Wee1\_a}} \text{Xic\_PCdk2\_CycE}$	
17	Phos_PCdk2_CycE	Phos_PCdk2_CycE	$\text{Cdk2\_CycE} \xrightarrow{\text{Wee1\_a}} \text{PCdk2\_CycE}$	
18	Kinase_regulation	Kinase _regulation	$\text{Cdk2\_CycE} \xrightarrow{\text{Cdk2\_CycE}} \text{Kin\_a} + \text{Cdk2\_CycE}$	
19	Xic_PCdk2_CycE_association	Xic_PCdk2_CycE_association	$\text{Xic} + \text{PCdk2\_CycE} \longrightarrow \text{Xic\_PCdk2\_CycE}$	
20	Xic_PCdk2_CycErem_association	Xic_PCdk2_CycErem_association	$\text{Xic} + \text{PCdk2\_CycErem} \longrightarrow \text{Xic\_PCdk2\_CycErem}$	
21	Xic_PCdk2_CycE_dissociation	Xic_PCdk2_CycE_dissociation	$\text{Xic\_PCdk2\_CycE} \longrightarrow \text{Xic} + \text{PCdk2\_CycE}$	
22	Xic_PCdk2_CycErem_dissociation	Xic_PCdk2_CycErem_dissociation	$\text{Xic\_PCdk2\_CycErem} \longrightarrow \text{Xic} + \text{PCdk2\_CycErem}$	

№	Id	Name	Reaction Equation	SBO
23	Degradation_Cdk2_CycErem	Degradation_Cdk2_CycErem	Cdk2_CycErem $\xrightarrow{\text{Deg\_a}} \emptyset$	
24	Degradation_PCdk2_CycErem	Degradation_PCdk2_CycErem	PCdk2_CycErem $\xrightarrow{\text{Deg\_a}} \emptyset$	
25	Xicrem_degradation	Xicrem degradation	Xicrem $\longrightarrow \emptyset$	
26	Xic_PCdk2_CycErem_to_not_rem	Xic_PCdk2_CycErem_to_not_rem	Xic_PCdk2_CycErem $\longrightarrow$ Xic_PCdk2_CycE	
27	Xic_Cdk2_CycErem_to_not_rem	Xic_Cdk2_CycErem_to_not_rem	Xic_Cdk2_CycErem $\longrightarrow$ Xic_Cdk2_CycE	
28	Xic_PCdk2_CycE_to_rem	Xic_PCdk2_CycE_to_rem	Xic_PCdk2_CycE $\longrightarrow$ Xic_PCdk2_CycErem	
29	Xic_Cdk2_CycE_to_rem	Xic_Cdk2_CycE_to_rem	Xic_Cdk2_CycE $\longrightarrow$ Xic_Cdk2_CycErem	
30	Wee1_regulation	Wee1_regulation	$\emptyset \xrightarrow{\text{Kin\_a, Wee1\_total}}$ Wee1_a	

8.1 Reaction Xic_Cdk2_CycE_association

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

Name Xic_Cdk2_CycE_association

Reaction equation

$$\text{Xic} + \text{Cdk2\_CycE} \longrightarrow \text{Xic\_Cdk2\_CycE} \tag{20}$$

Reactants

Table 6: Properties of each reactant.

Id	Name	SBO
Xic	Xic	
Cdk2_CycE	Cdk2_CycE	

Product

Table 7: Properties of each product.

Id	Name	SBO
Xic_Cdk2_CycE	Xic_Cdk2_CycE	

Kinetic Law

Derived unit $\text{s}^{-1} \cdot (0.0010\ \text{mol})^2 \cdot \text{ml}^{-1}$

$$v_1 = \text{vol}\,(\text{compartment}) \cdot \text{kassoc} \cdot [\text{Xic}] \cdot [\text{Cdk2\_CycE}] \tag{21}$$

8.2 Reaction Xic_Cdk2_CycErem_association

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

Name Xic_Cdk2_CycErem_association

Reaction equation

$$\text{Xic} + \text{Cdk2\_CycErem} \longrightarrow \text{Xic\_Cdk2\_CycErem} \tag{22}$$

Reactants

Table 8: Properties of each reactant.

Id	Name	SBO
Xic	Xic	
Cdk2_CycErem	Cdk2_CycErem	

Product

Table 9: Properties of each product.

Id	Name	SBO
Xic_Cdk2_CycErem	Xic_Cdk2_CycErem	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot (0.0010\ \mathrm{mol})^2 \cdot \mathrm{ml}^{-1}$

$$v_2 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{kassoc} \cdot [\mathrm{Xic}] \cdot [\mathrm{Cdk2\_CycErem}] \tag{23}$$

8.3 Reaction Xic_Cdk2_CycE_dissociation

This is an irreversible reaction of one reactant forming two products.

Name Xic_Cdk2_CycE_dissociation

Reaction equation

$$\mathrm{Xic\_Cdk2\_CycE} \longrightarrow \mathrm{Xic} + \mathrm{Cdk2\_CycE} \tag{24}$$

Reactant

Table 10: Properties of each reactant.

Id	Name	SBO
Xic_Cdk2_CycE	Xic_Cdk2_CycE	

Products

Table 11: Properties of each product.

Id	Name	SBO
Xic	Xic	
Cdk2_CycE	Cdk2_CycE	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{mmol}$

$$v_3 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{kdissoc} \cdot [\mathrm{Xic\_Cdk2\_CycE}] \tag{25}$$

8.4 Reaction Xic_Cdk2_CycErem_dissociation

This is an irreversible reaction of one reactant forming two products.

Name Xic_Cdk2_CycErem_dissociation

Reaction equation

$$\mathrm{Xic\_Cdk2\_CycErem} \longrightarrow \mathrm{Xic} + \mathrm{Cdk2\_CycErem} \tag{26}$$

Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
Xic_Cdk2_CycErem	Xic_Cdk2_CycErem	

Products

Table 13: Properties of each product.

Id	Name	SBO
Xic	Xic	
Cdk2_CycErem	Cdk2_CycErem	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{mmol}$

$$v_4 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{kdissoc} \cdot [\mathrm{Xic\_Cdk2\_CycErem}] \tag{27}$$

8.5 Reaction Cdk2_CycErem_to_not_rem

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

Name Cdk2_CycErem_to_not_rem

Reaction equation

$$\mathrm{Cdk2\_CycErem} \longrightarrow \mathrm{Cdk2\_CycE} \tag{28}$$

Reactant

Table 14: Properties of each reactant.

Id	Name	SBO
Cdk2_CycErem	Cdk2_CycErem	

Product

Table 15: Properties of each product.

Id	Name	SBO
Cdk2_CycE	Cdk2_CycE	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{mmol}$

$$v_5 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{koff} \cdot [\mathrm{Cdk2\_CycErem}] \tag{29}$$

8.6 Reaction PCdk2_CycE_to_not_rem

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

Name PCdk2_CycE_to_not_rem

Reaction equation

$$\mathrm{PCdk2\_CycErem} \longrightarrow \mathrm{PCdk2\_CycE} \tag{30}$$

Reactant

Table 16: Properties of each reactant.

Id	Name	SBO
PCdk2_CycErem	PCdk2_CycErem	

Product

Table 17: Properties of each product.

Id	Name	SBO
PCdk2_CycE	PCdk2_CycE	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{mmol}$

$$v_6 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{koff} \cdot [\mathrm{PCdk2\_CycErem}] \tag{31}$$

8.7 Reaction Cdk2_CycE_to_rem

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

Name Cdk2_CycE_to_rem

Reaction equation

$$\mathrm{Cdk2\_CycE} \longrightarrow \mathrm{Cdk2\_CycErem} \tag{32}$$

Reactant

Table 18: Properties of each reactant.

Id	Name	SBO
Cdk2_CycE	Cdk2_CycE	

Product

Table 19: Properties of each product.

Id	Name	SBO
Cdk2_CycErem	Cdk2_CycErem	

Kinetic Law

Derived unit $s^{-1} \cdot mmol$

$$v_7 = \text{vol}(\text{compartment}) \cdot \text{function\_removed\_from\_oscillatory\_system\_1}([\text{Cdk2\_CycE}], \text{kon}, \text{phi}) \tag{33}$$

$$\text{function\_removed\_from\_oscillatory\_system\_1}([\text{Cdk2\_CycE}], \text{kon}, \text{phi}) = \text{kon} \cdot \text{phi} \cdot [\text{Cdk2\_CycE}] \tag{34}$$

$$\text{function\_removed\_from\_oscillatory\_system\_1}([\text{Cdk2\_CycE}], \text{kon}, \text{phi}) = \text{kon} \cdot \text{phi} \cdot [\text{Cdk2\_CycE}] \tag{35}$$

8.8 Reaction PCdk2_CycE_to_rem

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

Name PCdk2_CycE_to_rem

Reaction equation

$$\text{PCdk2\_CycE} \longrightarrow \text{PCdk2\_CycErem} \tag{36}$$

Reactant

Table 20: Properties of each reactant.

Id	Name	SBO
PCdk2_CycE	PCdk2_CycE	

Product

Table 21: Properties of each product.

Id	Name	SBO
PCdk2_CycErem	PCdk2_CycErem	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{mmol}$

$$v_8 = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{function\_removed\_from\_oscillatory\_system\_2}\,([\mathrm{PCdk2\_CycE}], \mathrm{kon}, \mathrm{phi}) \tag{37}$$

$$\mathrm{function\_removed\_from\_oscillatory\_system\_2}\,([\mathrm{PCdk2\_CycE}], \mathrm{kon}, \mathrm{phi}) = \mathrm{kon} \cdot \mathrm{phi} \cdot [\mathrm{PCdk2\_CycE}] \tag{38}$$

$$\mathrm{function\_removed\_from\_oscillatory\_system\_2}\,([\mathrm{PCdk2\_CycE}], \mathrm{kon}, \mathrm{phi}) = \mathrm{kon} \cdot \mathrm{phi} \cdot [\mathrm{PCdk2\_CycE}] \tag{39}$$

8.9 Reaction X_degadation

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

Name X_degadation

Reaction equation

$$\mathrm{Xic\_Cdk2\_CycErem} \longrightarrow \mathrm{Cdk2\_CycErem} \tag{40}$$

Reactant

Table 22: Properties of each reactant.

Id	Name	SBO
Xic_Cdk2_CycErem	Xic_Cdk2_CycErem	

Product

Table 23: Properties of each product.

Id	Name	SBO
Cdk2_CycErem	Cdk2_CycErem	

Kinetic Law

Derived unit $s^{-1} \cdot mmol$

$$v_9 = \text{vol}(\text{compartment}) \cdot \text{kxdeg} \cdot [\text{Xic\_Cdk2\_CycErem}] \tag{41}$$

8.10 Reaction X_degradation_phosphorylated_complex

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

Name X_degradation_phosphorylated_complex

Reaction equation

$$\text{Xic\_PCdk2\_CycErem} \longrightarrow \text{PCdk2\_CycErem} \tag{42}$$

Reactant

Table 24: Properties of each reactant.

Id	Name	SBO
Xic_PCdk2_CycErem	Xic_PCdk2_CycErem	

Product

Table 25: Properties of each product.

Id	Name	SBO
PCdk2_CycErem	PCdk2_CycErem	

Kinetic Law

Derived unit $s^{-1} \cdot mmol$

$$v_{10} = \text{vol}(\text{compartment}) \cdot \text{kxdeg} \cdot [\text{Xic\_PCdk2\_CycErem}] \tag{43}$$

8.11 Reaction Degradation_XicPCdk2_CycErem

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

Name Degradation_XicPCdk2_CycErem

Reaction equation

$$\text{Xic\_PCdk2\_CycErem} \xrightarrow{\text{Deg\_a}} \text{Xicrem} \tag{44}$$

Reactant

Table 26: Properties of each reactant.

Id	Name	SBO
Xic_PCdk2_CycErem	Xic_PCdk2_CycErem	

Modifier

Table 27: Properties of each modifier.

Id	Name	SBO
Deg_a	Deg_CycE	

Product

Table 28: Properties of each product.

Id	Name	SBO
Xicrem	Xicrem	

Kinetic Law

Derived unit $(0.0010\,\mathrm{l})^{-1} \cdot \mathrm{s}^{-1} \cdot (0.0010\,\mathrm{mol})^{2}$

$$v_{11} = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{Function\_for\_degradation\_of\_Xic\_Cyc\_Cdk\_1}\,([\mathrm{Deg\_a}], [\mathrm{Xic\_PCdk2\_CycErem}], \mathrm{kedeg}) \tag{45}$$

$$\text{Function\_for\_degradation\_of\_Xic\_Cyc\_Cdk\_1}([\text{Deg\_a}], [\text{Xic\_PCdk2\_CycErem}], \text{kedeg}) = \text{kedeg} \cdot [\text{Xic\_PCdk2\_CycErem}] \cdot [\text{Deg\_a}] \tag{46}$$

$$\text{Function\_for\_degradation\_of\_Xic\_Cyc\_Cdk\_1}([\text{Deg\_a}], [\text{Xic\_PCdk2\_CycErem}], \text{kedeg}) = \text{kedeg} \cdot [\text{Xic\_PCdk2\_CycErem}] \cdot [\text{Deg\_a}] \tag{47}$$

8.12 Reaction `Degradation_XicCdk2_CycErem`

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

Name Degradation_XicCdk2_CycErem

Reaction equation

$$\text{Xic\_Cdk2\_CycErem} \xrightarrow{\text{Deg\_a}} \text{Xicrem} \tag{48}$$

Reactant

Table 29: Properties of each reactant.

Id	Name	SBO
`Xic_Cdk2_CycErem`	Xic_Cdk2_CycErem	

Modifier

Table 30: Properties of each modifier.

Id	Name	SBO
`Deg_a`	Deg_CycE	

Product

Table 31: Properties of each product.

Id	Name	SBO
`Xicrem`	Xicrem	

Kinetic Law

Derived unit $(0.0010\,\mathrm{l})^{-1} \cdot \mathrm{s}^{-1} \cdot (0.0010\,\mathrm{mol})^{2}$

$$v_{12} = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{Function\_for\_degradation\_of\_Xic\_Cyc\_Cdk\_2}\,([\mathrm{Deg\_a}], [\mathrm{Xic\_Cdk2\_CycErem}], \mathrm{kedeg}) \tag{49}$$

$$\mathrm{Function\_for\_degradation\_of\_Xic\_Cyc\_Cdk\_2}\,([\mathrm{Deg\_a}], [\mathrm{Xic\_Cdk2\_CycErem}], \mathrm{kedeg}) = \mathrm{kedeg} \cdot [\mathrm{Xic\_Cdk2\_CycErem}] \cdot [\mathrm{Deg\_a}] \tag{50}$$

$$\mathrm{Function\_for\_degradation\_of\_Xic\_Cyc\_Cdk\_2}\,([\mathrm{Deg\_a}], [\mathrm{Xic\_Cdk2\_CycErem}], \mathrm{kedeg}) = \mathrm{kedeg} \cdot [\mathrm{Xic\_Cdk2\_CycErem}] \cdot [\mathrm{Deg\_a}] \tag{51}$$

8.13 Reaction `Dephos_Xic_PCdk2_CycE`

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

Name Dephos_Xic_PCdk2_CycE

Reaction equation

$$\mathrm{Xic\_PCdk2\_CycE} \longrightarrow \mathrm{Xic\_Cdk2\_CycE} \tag{52}$$

Reactant

Table 32: Properties of each reactant.

Id	Name	SBO
`Xic_PCdk2_CycE`	Xic_PCdk2_CycE	

Product

Table 33: Properties of each product.

Id	Name	SBO
`Xic_Cdk2_CycE`	Xic_Cdk2_CycE	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{mmol}$

$$v_{13} = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{k25A} \cdot [\mathrm{Xic\_PCdk2\_CycE}] \tag{53}$$

8.14 Reaction `Dephos_PCdk2_CycE`

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

Name Dephos_PCdk2_CycE

Reaction equation

$$\mathrm{PCdk2\_CycE} \longrightarrow \mathrm{Cdk2\_CycE} \tag{54}$$

Reactant

Table 34: Properties of each reactant.

Id	Name	SBO
`PCdk2_CycE`	PCdk2_CycE	

Product

Table 35: Properties of each product.

Id	Name	SBO
`Cdk2_CycE`	Cdk2_CycE	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{mmol}$

$$v_{14} = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{k25A} \cdot [\mathrm{PCdk2\_CycE}] \tag{55}$$

8.15 Reaction `Degradation_increase`

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

Name Degradation_increase

Reaction equation

$$\emptyset \longrightarrow \text{Deg\_a} \tag{56}$$

Product

Table 36: Properties of each product.

Id	Name	SBO
Deg_a	Deg_CycE	

Kinetic Law

Derived unit $\text{ml} \cdot \text{s}^{-1}$

$$v_{15} = \text{vol}\,(\text{compartment}) \cdot \text{function\_Hill\_Cdk2\_CycE\_removal\_1}\,(\text{Heav}, \text{kdact}) \tag{57}$$

$$\text{function\_Hill\_Cdk2\_CycE\_removal\_1}\,(\text{Heav}, \text{kdact}) = \text{kdact} \cdot \text{Heav} \tag{58}$$

$$\text{function\_Hill\_Cdk2\_CycE\_removal\_1}\,(\text{Heav}, \text{kdact}) = \text{kdact} \cdot \text{Heav} \tag{59}$$

8.16 Reaction Phos_Xic_PCdk2_CycE

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

Name Phos_Xic_PCdk2_CycE

Reaction equation

$$\text{Xic\_Cdk2\_CycE} \xrightarrow{\text{Wee1\_a}} \text{Xic\_PCdk2\_CycE} \tag{60}$$

Reactant

Table 37: Properties of each reactant.

Id	Name	SBO
Xic_Cdk2_CycE	Xic_Cdk2_CycE	

Modifier

Table 38: Properties of each modifier.

Id	Name	SBO
Wee1_a	Wee1_a	

Product

Table 39: Properties of each product.

Id	Name	SBO
Xic_PCdk2_CycE	Xic_PCdk2_CycE	

Kinetic Law

Derived unit $(0.0010\,\mathrm{l})^{-1} \cdot \mathrm{s}^{-1} \cdot (0.0010\,\mathrm{mol})^{2}$

$$v_{16} = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{Function\_phosphorylation\_with\_Wee1\_1}\,([\mathrm{Wee1\_a}], [\mathrm{Xic\_Cdk2\_CycE}], \mathrm{kwee}) \tag{61}$$

$$\mathrm{Function\_phosphorylation\_with\_Wee1\_1}\,([\mathrm{Wee1\_a}], [\mathrm{Xic\_Cdk2\_CycE}], \mathrm{kwee}) = \mathrm{kwee} \cdot [\mathrm{Wee1\_a}] \cdot [\mathrm{Xic\_Cdk2\_CycE}] \tag{62}$$

$$\mathrm{Function\_phosphorylation\_with\_Wee1\_1}\,([\mathrm{Wee1\_a}], [\mathrm{Xic\_Cdk2\_CycE}], \mathrm{kwee}) = \mathrm{kwee} \cdot [\mathrm{Wee1\_a}] \cdot [\mathrm{Xic\_Cdk2\_CycE}] \tag{63}$$

8.17 Reaction Phos_PCdk2_CycE

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

Name Phos_PCdk2_CycE

Reaction equation

$$\mathrm{Cdk2\_CycE} \xrightarrow{\mathrm{Wee1\_a}} \mathrm{PCdk2\_CycE} \tag{64}$$

Reactant

Table 40: Properties of each reactant.

Id	Name	SBO
Cdk2_CycE	Cdk2_CycE	

Modifier

Table 41: Properties of each modifier.

Id	Name	SBO
Wee1_a	Wee1_a	

Product

Table 42: Properties of each product.

Id	Name	SBO
PCdk2_CycE	PCdk2_CycE	

Kinetic Law

Derived unit $(0.0010\,\mathrm{l})^{-1} \cdot \mathrm{s}^{-1} \cdot (0.0010\,\mathrm{mol})^{2}$

$$v_{17} = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{Function\_phosphorylation\_with\_Wee1\_2}\,([\mathrm{Cdk2\_CycE}], [\mathrm{Wee1\_a}], \mathrm{kwee}) \tag{65}$$

$$\mathrm{Function\_phosphorylation\_with\_Wee1\_2}\,([\mathrm{Cdk2\_CycE}], [\mathrm{Wee1\_a}], \mathrm{kwee}) = \mathrm{kwee} \cdot [\mathrm{Wee1\_a}] \cdot [\mathrm{Cdk2\_CycE}] \tag{66}$$

$$\mathrm{Function\_phosphorylation\_with\_Wee1\_2}\,([\mathrm{Cdk2\_CycE}], [\mathrm{Wee1\_a}], \mathrm{kwee}) = \mathrm{kwee} \cdot [\mathrm{Wee1\_a}] \cdot [\mathrm{Cdk2\_CycE}] \tag{67}$$

8.18 Reaction Kinase__regulation

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

Name Kinase _regulation

Reaction equation

$$\text{Cdk2\_CycE} \xrightarrow{\text{Cdk2\_CycE}} \text{Kin\_a} + \text{Cdk2\_CycE} \tag{68}$$

Reactant

Table 43: Properties of each reactant.

Id	Name	SBO
Cdk2_CycE	Cdk2_CycE	

Modifier

Table 44: Properties of each modifier.

Id	Name	SBO
Cdk2_CycE	Cdk2_CycE	

Products

Table 45: Properties of each product.

Id	Name	SBO
Kin_a	Kin_a	
Cdk2_CycE	Cdk2_CycE	

Kinetic Law

Derived unit contains undeclared units

$$\begin{aligned} v_{18} = {} & \text{vol}\,(\text{compartment}) \\ & \cdot \text{Function\_for\_Kin\_a\_1}\,([\text{Cdk2\_CycE}], \text{Jiact}, \text{Jiinact}, [\text{Kin\_a}], \text{kiact}, \text{kiinact}) \end{aligned} \tag{69}$$

$$\begin{aligned} & \text{Function\_for\_Kin\_a\_1}\,([\text{Cdk2\_CycE}], \text{Jiact}, \text{Jiinact}, [\text{Kin\_a}], \text{kiact}, \text{kiinact}) \\ & = \frac{\text{kiact} \cdot (1 - [\text{Kin\_a}])}{\text{Jiact} + 1 - [\text{Kin\_a}]} - \frac{\text{kiinact} \cdot [\text{Cdk2\_CycE}] \cdot [\text{Kin\_a}]}{\text{Jiinact} + [\text{Kin\_a}]} \end{aligned} \tag{70}$$

$$\begin{aligned}&\text{Function\_for\_Kin\_a\_1}\left([\text{Cdk2\_CycE}], \text{Jiact}, \text{Jiinact}, [\text{Kin\_a}], \text{kiact}, \text{kiinact}\right)\\&= \frac{\text{kiact} \cdot (1 - [\text{Kin\_a}])}{\text{Jiact} + 1 - [\text{Kin\_a}]} - \frac{\text{kiinact} \cdot [\text{Cdk2\_CycE}] \cdot [\text{Kin\_a}]}{\text{Jiinact} + [\text{Kin\_a}]}\end{aligned} \tag{71}$$

8.19 Reaction `Xic_PCdk2_CycE_association`

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

Name Xic_PCdk2_CycE_association

Reaction equation

$$\text{Xic} + \text{PCdk2\_CycE} \longrightarrow \text{Xic\_PCdk2\_CycE} \tag{72}$$

Reactants

Table 46: Properties of each reactant.

Id	Name	SBO
`Xic`	Xic	
`PCdk2_CycE`	PCdk2_CycE	

Product

Table 47: Properties of each product.

Id	Name	SBO
`Xic_PCdk2_CycE`	Xic_PCdk2_CycE	

Kinetic Law

Derived unit $\text{s}^{-1} \cdot (0.0010\ \text{mol})^2 \cdot \text{ml}^{-1}$

$$v_{19} = \text{vol}\left(\text{compartment}\right) \cdot \text{kassoc} \cdot [\text{Xic}] \cdot [\text{PCdk2\_CycE}] \tag{73}$$

8.20 Reaction `Xic_PCdk2_CycErem_association`

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

Name Xic_PCdk2_CycErem_association

Reaction equation

$$\text{Xic} + \text{PCdk2\_CycErem} \longrightarrow \text{Xic\_PCdk2\_CycErem} \tag{74}$$

Reactants

Table 48: Properties of each reactant.

Id	Name	SBO
`Xic`	Xic	
`PCdk2_CycErem`	PCdk2_CycErem	

Product

Table 49: Properties of each product.

Id	Name	SBO
`Xic_PCdk2_CycErem`	Xic_PCdk2_CycErem	

Kinetic Law

Derived unit $\text{s}^{-1} \cdot (0.0010\ \text{mol})^2 \cdot \text{ml}^{-1}$

$$v_{20} = \text{vol}\,(\text{compartment}) \cdot \text{kassoc} \cdot [\text{Xic}] \cdot [\text{PCdk2\_CycErem}] \tag{75}$$

8.21 Reaction `Xic_PCdk2_CycE_dissociation`

This is an irreversible reaction of one reactant forming two products.

Name Xic_PCdk2_CycE_dissociation

Reaction equation

$$\text{Xic\_PCdk2\_CycE} \longrightarrow \text{Xic} + \text{PCdk2\_CycE} \tag{76}$$

Reactant

Table 50: Properties of each reactant.

Id	Name	SBO
Xic_PCdk2_CycE	Xic_PCdk2_CycE	

Products

Table 51: Properties of each product.

Id	Name	SBO
Xic	Xic	
PCdk2_CycE	PCdk2_CycE	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{mmol}$

$$v_{21} = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{kdissoc} \cdot [\mathrm{Xic\_PCdk2\_CycE}] \tag{77}$$

8.22 Reaction Xic_PCdk2_CycErem_dissociation

This is an irreversible reaction of one reactant forming two products.

Name Xic_PCdk2_CycErem_dissociation

Reaction equation

$$\mathrm{Xic\_PCdk2\_CycErem} \longrightarrow \mathrm{Xic} + \mathrm{PCdk2\_CycErem} \tag{78}$$

Reactant

Table 52: Properties of each reactant.

Id	Name	SBO
Xic_PCdk2_CycErem	Xic_PCdk2_CycErem	

Products

Table 53: Properties of each product.

Id	Name	SBO
Xic	Xic	
PCdk2_CycErem	PCdk2_CycErem	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{mmol}$

$$v_{22} = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{kdissoc} \cdot [\mathrm{Xic\_PCdk2\_CycErem}] \tag{79}$$

8.23 Reaction Degradation_Cdk2_CycErem

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

Name Degradation_Cdk2_CycErem

Reaction equation

$$\mathrm{Cdk2\_CycErem} \xrightarrow{\mathrm{Deg\_a}} \emptyset \tag{80}$$

Reactant

Table 54: Properties of each reactant.

Id	Name	SBO
Cdk2_CycErem	Cdk2_CycErem	

Modifier

Table 55: Properties of each modifier.

Id	Name	SBO
Deg_a	Deg_CycE	

Kinetic Law

Derived unit $(0.0010\,\mathrm{l})^{-1} \cdot \mathrm{s}^{-1} \cdot (0.0010\,\mathrm{mol})^{2}$

$$v_{23} = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{Function\_for\_degradation\_of\_Xic\_Cyc\_Cdk\_3}\,([\mathrm{Cdk2\_CycErem}], [\mathrm{Deg\_a}], \mathrm{kedeg}) \tag{81}$$

$$\mathrm{Function\_for\_degradation\_of\_Xic\_Cyc\_Cdk\_3}\,([\mathrm{Cdk2\_CycErem}], [\mathrm{Deg\_a}], \mathrm{kedeg}) = \mathrm{kedeg} \cdot [\mathrm{Cdk2\_CycErem}] \cdot [\mathrm{Deg\_a}] \tag{82}$$

$$\mathrm{Function\_for\_degradation\_of\_Xic\_Cyc\_Cdk\_3}\,([\mathrm{Cdk2\_CycErem}], [\mathrm{Deg\_a}], \mathrm{kedeg}) = \mathrm{kedeg} \cdot [\mathrm{Cdk2\_CycErem}] \cdot [\mathrm{Deg\_a}] \tag{83}$$

8.24 Reaction `Degradation_PCdk2_CycErem`

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

Name Degradation_PCdk2_CycErem

Reaction equation

$$\mathrm{PCdk2\_CycErem} \xrightarrow{\mathrm{Deg\_a}} \emptyset \tag{84}$$

Reactant

Table 56: Properties of each reactant.

Id	Name	SBO
`PCdk2_CycErem`	PCdk2_CycErem	

Modifier

Table 57: Properties of each modifier.

Id	Name	SBO
`Deg_a`	Deg_CycE	

Kinetic Law

Derived unit $(0.0010\,\mathrm{l})^{-1} \cdot \mathrm{s}^{-1} \cdot (0.0010\,\mathrm{mol})^{2}$

$$v_{24} = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{Function\_for\_degradation\_of\_Xic\_Cyc\_Cdk\_4}\,([\mathrm{Deg\_a}], [\mathrm{PCdk2\_CycErem}], \mathrm{kedeg}) \tag{85}$$

$$\mathrm{Function\_for\_degradation\_of\_Xic\_Cyc\_Cdk\_4}\,([\mathrm{Deg\_a}], [\mathrm{PCdk2\_CycErem}], \mathrm{kedeg}) = \mathrm{kedeg} \cdot [\mathrm{PCdk2\_CycErem}] \cdot [\mathrm{Deg\_a}] \tag{86}$$

$$\mathrm{Function\_for\_degradation\_of\_Xic\_Cyc\_Cdk\_4}\,([\mathrm{Deg\_a}], [\mathrm{PCdk2\_CycErem}], \mathrm{kedeg}) = \mathrm{kedeg} \cdot [\mathrm{PCdk2\_CycErem}] \cdot [\mathrm{Deg\_a}] \tag{87}$$

8.25 Reaction `Xicrem_degradation`

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

Name Xicrem degradation

Reaction equation

$$\mathrm{Xicrem} \longrightarrow \emptyset \tag{88}$$

Reactant

Table 58: Properties of each reactant.

Id	Name	SBO
`Xicrem`	Xicrem	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{mmol}$

$$v_{25} = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{kxdeg} \cdot [\mathrm{Xicrem}] \tag{89}$$

8.26 Reaction `Xic_PCdk2_CycErem_to_not_rem`

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

Name Xic_PCdk2_CycErem_to_not_rem

Reaction equation

$$\mathrm{Xic\_PCdk2\_CycErem} \longrightarrow \mathrm{Xic\_PCdk2\_CycE} \tag{90}$$

Reactant

Table 59: Properties of each reactant.

Id	Name	SBO
Xic_PCdk2_CycErem	Xic_PCdk2_CycErem	

Product

Table 60: Properties of each product.

Id	Name	SBO
Xic_PCdk2_CycE	Xic_PCdk2_CycE	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{mmol}$

$$v_{26} = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{koff} \cdot [\mathrm{Xic\_PCdk2\_CycErem}] \tag{91}$$

8.27 Reaction Xic_Cdk2_CycErem_to_not_rem

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

Name Xic_Cdk2_CycErem_to_not_rem

Reaction equation

$$\mathrm{Xic\_Cdk2\_CycErem} \longrightarrow \mathrm{Xic\_Cdk2\_CycE} \tag{92}$$

Reactant

Table 61: Properties of each reactant.

Id	Name	SBO
Xic_Cdk2_CycErem	Xic_Cdk2_CycErem	

Product

Table 62: Properties of each product.

Id	Name	SBO
Xic_Cdk2_CycE	Xic_Cdk2_CycE	

Kinetic Law

Derived unit $s^{-1} \cdot mmol$

$$v_{27} = \text{vol}(\text{compartment}) \cdot \text{koff} \cdot [\text{Xic\_Cdk2\_CycErem}] \tag{93}$$

8.28 Reaction Xic_PCdk2_CycE_to_rem

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

Name Xic_PCdk2_CycE_to_rem

Reaction equation

$$\text{Xic\_PCdk2\_CycE} \longrightarrow \text{Xic\_PCdk2\_CycErem} \tag{94}$$

Reactant

Table 63: Properties of each reactant.

Id	Name	SBO
Xic_PCdk2_CycE	Xic_PCdk2_CycE	

Product

Table 64: Properties of each product.

Id	Name	SBO
Xic_PCdk2_CycErem	Xic_PCdk2_CycErem	

Kinetic Law

Derived unit $s^{-1} \cdot mmol$

$$v_{28} = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{function\_removed\_from\_oscillatory\_system\_3}\,([\mathrm{Xic\_PCdk2\_CycE}], \mathrm{kon}, \mathrm{phi}) \tag{95}$$

$$\mathrm{function\_removed\_from\_oscillatory\_system\_3}\,([\mathrm{Xic\_PCdk2\_CycE}], \mathrm{kon}, \mathrm{phi}) = \mathrm{kon} \cdot \mathrm{phi} \cdot [\mathrm{Xic\_PCdk2\_CycE}] \tag{96}$$

$$\mathrm{function\_removed\_from\_oscillatory\_system\_3}\,([\mathrm{Xic\_PCdk2\_CycE}], \mathrm{kon}, \mathrm{phi}) = \mathrm{kon} \cdot \mathrm{phi} \cdot [\mathrm{Xic\_PCdk2\_CycE}] \tag{97}$$

8.29 Reaction `Xic_Cdk2_CycE_to_rem`

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

Name Xic_Cdk2_CycE_to_rem

Reaction equation

$$\mathrm{Xic\_Cdk2\_CycE} \longrightarrow \mathrm{Xic\_Cdk2\_CycErem} \tag{98}$$

Reactant

Table 65: Properties of each reactant.

Id	Name	SBO
`Xic_Cdk2_CycE`	Xic_Cdk2_CycE	

Product

Table 66: Properties of each product.

Id	Name	SBO
`Xic_Cdk2_CycErem`	Xic_Cdk2_CycErem	

Kinetic Law

Derived unit $\mathrm{s}^{-1} \cdot \mathrm{mmol}$

$$v_{29} = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{function\_removed\_from\_oscillatory\_system\_4}\,([\mathrm{Xic\_Cdk2\_CycE}], \mathrm{kon}, \mathrm{phi}) \tag{99}$$

$$\mathrm{function\_removed\_from\_oscillatory\_system\_4}\,([\mathrm{Xic\_Cdk2\_CycE}], \mathrm{kon}, \mathrm{phi}) = \mathrm{kon} \cdot \mathrm{phi} \cdot [\mathrm{Xic\_Cdk2\_CycE}] \tag{100}$$

$$\mathrm{function\_removed\_from\_oscillatory\_system\_4}\,([\mathrm{Xic\_Cdk2\_CycE}], \mathrm{kon}, \mathrm{phi}) = \mathrm{kon} \cdot \mathrm{phi} \cdot [\mathrm{Xic\_Cdk2\_CycE}] \tag{101}$$

8.30 Reaction `Wee1_regulation`

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

Name Wee1_regulation

Reaction equation

$$\emptyset \xrightarrow{\mathrm{Kin\_a,\ Wee1\_total}} \mathrm{Wee1\_a} \tag{102}$$

Modifiers

Table 67: Properties of each modifier.

Id	Name	SBO
`Kin_a`	Kin_a	
`Wee1_total`	Wee1_total	

Product

Table 68: Properties of each product.

Id	Name	SBO
`Wee1_a`	Wee1_a	

Kinetic Law

Derived unit contains undeclared units

$$v_{30} = \mathrm{vol}\,(\mathrm{compartment}) \cdot \mathrm{Function\_for\_Wee1\_a\_1}\,(\mathrm{Jwact}, \mathrm{Jwinact}, [\mathrm{Kin\_a}], [\mathrm{Wee1\_a}], [\mathrm{Wee1\_total}], \mathrm{kwact}, \mathrm{kwinact}) \tag{103}$$

$$\mathrm{Function\_for\_Wee1\_a\_1}\,(\mathrm{Jwact}, \mathrm{Jwinact}, [\mathrm{Kin\_a}], [\mathrm{Wee1\_a}], [\mathrm{Wee1\_total}], \mathrm{kwact}, \mathrm{kwinact}) = \frac{\mathrm{kwact} \cdot ([\mathrm{Wee1\_total}] - [\mathrm{Wee1\_a}])}{\mathrm{Jwact} + [\mathrm{Wee1\_total}] - [\mathrm{Wee1\_a}]} - \frac{\mathrm{kwinact} \cdot [\mathrm{Kin\_a}] \cdot [\mathrm{Wee1\_a}]}{\mathrm{Jwinact} + [\mathrm{Wee1\_a}]} \tag{104}$$

$$\mathrm{Function\_for\_Wee1\_a\_1}\,(\mathrm{Jwact}, \mathrm{Jwinact}, [\mathrm{Kin\_a}], [\mathrm{Wee1\_a}], [\mathrm{Wee1\_total}], \mathrm{kwact}, \mathrm{kwinact}) = \frac{\mathrm{kwact} \cdot ([\mathrm{Wee1\_total}] - [\mathrm{Wee1\_a}])}{\mathrm{Jwact} + [\mathrm{Wee1\_total}] - [\mathrm{Wee1\_a}]} - \frac{\mathrm{kwinact} \cdot [\mathrm{Kin\_a}] \cdot [\mathrm{Wee1\_a}]}{\mathrm{Jwinact} + [\mathrm{Wee1\_a}]} \tag{105}$$

9 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.

9.1 Species PCdk2_CycE

Name PCdk2_CycE

Initial concentration $0.94\ \mathrm{mmol} \cdot \mathrm{ml}^{-1}$

This species takes part in six reactions (as a reactant in PCdk2_CycE_to_rem, Dephos_PCdk2_CycE, Xic_PCdk2_CycE_association and as a product in PCdk2_CycE_to_not_rem, Phos_PCdk2_CycE, Xic_PCdk2_CycE_dissociation).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{PCdk2\_CycE} = v_6 + v_{17} + v_{21} - v_8 - v_{14} - v_{19} \tag{106}$$

9.2 Species Cdk2_CycE

Name Cdk2_CycE

Initial concentration $0.0599999999999999\ \mathrm{mmol} \cdot \mathrm{ml}^{-1}$

This species takes part in nine reactions (as a reactant in Xic_Cdk2_CycE_association, Cdk2_CycE_to_rem, Phos_PCdk2_CycE, Kinase__regulation and as a product in Xic_Cdk2_CycE_dissociation, Cdk2_CycErem_to_not_rem, Dephos_PCdk2_CycE, Kinase__regulation and as a modifier in Kinase__regulation).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Cdk2\_CycE} = v_3 + v_5 + v_{14} + v_{18} - v_1 - v_7 - v_{17} - v_{18} \tag{107}$$

9.3 Species Wee1_a

Name Wee1_a

Initial concentration $1.02\ \mathrm{mmol \cdot ml^{-1}}$

This species takes part in three reactions (as a product in Wee1_regulation and as a modifier in Phos_Xic_PCdk2_CycE, Phos_PCdk2_CycE).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Wee1\_a} = v_{30} \tag{108}$$

9.4 Species Wee1_total

Name Wee1_total

Initial concentration $7.99999999999998\ \mathrm{mmol \cdot ml^{-1}}$

This species takes part in one reaction (as a modifier in Wee1_regulation), which does not influence its rate of change because this constant species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Wee1\_total} = 0 \tag{109}$$

9.5 Species Cdk2_CycErem

Name Cdk2_CycErem

Initial concentration $0\ \mathrm{mmol \cdot ml^{-1}}$

This species takes part in six reactions (as a reactant in Xic_Cdk2_CycErem_association, Cdk2_CycErem_to_not_rem, Degradation_Cdk2_CycErem and as a product in Xic_Cdk2_CycErem_dissociation, Cdk2_CycE_to_rem, X_degadation).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Cdk2\_CycErem} = v_4 + v_7 + v_9 - v_2 - v_5 - v_{23} \tag{110}$$

9.6 Species PCdk2_CycErem

Name PCdk2_CycErem

Initial concentration $0\ \mathrm{mmol}\cdot\mathrm{ml}^{-1}$

This species takes part in six reactions (as a reactant in PCdk2_CycE_to_not_rem, Xic_PCdk2_CycErem_association, Degradation_PCdk2_CycErem and as a product in PCdk2_CycE_to_rem, X_degradation_phosphorylated_complex, Xic_PCdk2_CycErem_dissociation).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{PCdk2\_CycErem} = v_8 + v_{10} + v_{22} - v_6 - v_{20} - v_{24} \tag{111}$$

9.7 Species Deg_a

Name Deg_CycE

Initial concentration $0\ \mathrm{mmol}\cdot\mathrm{ml}^{-1}$

This species takes part in five reactions (as a product in Degradation_increase and as a modifier in Degradation_XicPCdk2_CycErem, Degradation_XicCdk2_CycErem, Degradation_Cdk2_CycErem, Degradation_PCdk2_CycErem).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Deg\_a} = v_{15} \tag{112}$$

9.8 Species Xic

Name Xic

Initial concentration $2.99999999999998\ \mathrm{mmol}\cdot\mathrm{ml}^{-1}$

This species takes part in eight reactions (as a reactant in Xic_Cdk2_CycE_association, Xic_Cdk2_CycErem_association, Xic_PCdk2_CycE_association, Xic_PCdk2_CycErem_association and as a product in Xic_Cdk2_CycE_dissociation, Xic_Cdk2_CycErem_dissociation, Xic_PCdk2_CycE_dissociation, Xic_PCdk2_CycErem_dissociation).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Xic} = v_3 + v_4 + v_{21} + v_{22} - v_1 - v_2 - v_{19} - v_{20} \tag{113}$$

9.9 Species Xic_Cdk2_CycE

Name Xic_Cdk2_CycE

Initial concentration $0\ \mathrm{mmol}\cdot\mathrm{ml}^{-1}$

This species takes part in six reactions (as a reactant in Xic_Cdk2_CycE_dissociation, Phos_Xic_PCdk2_CycE, Xic_Cdk2_CycE_to_rem and as a product in Xic_Cdk2_CycE_association, Dephos_Xic_PCdk2_CycE, Xic_Cdk2_CycErem_to_not_rem).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Xic\_Cdk2\_CycE} = v_1 + v_{13} + v_{27} - v_3 - v_{16} - v_{29} \tag{114}$$

9.10 Species Xic_PCdk2_CycE

Name Xic_PCdk2_CycE

Initial concentration $0\ \mathrm{mmol}\cdot\mathrm{ml}^{-1}$

This species takes part in six reactions (as a reactant in Dephos_Xic_PCdk2_CycE, Xic_PCdk2-_CycE_dissociation, Xic_PCdk2_CycE_to_rem and as a product in Phos_Xic_PCdk2_CycE, Xic_PCdk2_CycE_association, Xic_PCdk2_CycErem_to_not_rem).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Xic\_PCdk2\_CycE} = v_{16} + v_{19} + v_{26} - v_{13} - v_{21} - v_{28} \tag{115}$$

9.11 Species Xic_Cdk2_CycErem

Name Xic_Cdk2_CycErem

Initial concentration $0\ \mathrm{mmol}\cdot\mathrm{ml}^{-1}$

This species takes part in six reactions (as a reactant in Xic_Cdk2_CycErem_dissociation, X_degadation, Degradation_XicCdk2_CycErem, Xic_Cdk2_CycErem_to_not_rem and as a product in Xic_Cdk2_CycErem_association, Xic_Cdk2_CycE_to_rem).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Xic\_Cdk2\_CycErem} = v_{2} + v_{29} - v_{4} - v_{9} - v_{12} - v_{27} \tag{116}$$

9.12 Species Xic_PCdk2_CycErem

Name Xic_PCdk2_CycErem

Initial concentration $0\ \mathrm{mmol}\cdot\mathrm{ml}^{-1}$

This species takes part in six reactions (as a reactant in X_degradation_phosphorylated-_complex, Degradation_XicPCdk2_CycErem, Xic_PCdk2_CycErem_dissociation, Xic_PCdk2-_CycErem_to_not_rem and as a product in Xic_PCdk2_CycErem_association, Xic_PCdk2-_CycE_to_rem).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Xic\_PCdk2\_CycErem} = v_{20} + v_{28} - v_{10} - v_{11} - v_{22} - v_{26} \tag{117}$$

9.13 Species Xicrem

Name Xicrem

Initial concentration $0\ \mathrm{mmol}\cdot\mathrm{ml}^{-1}$

This species takes part in three reactions (as a reactant in Xicrem_degradation and as a product in Degradation_XicPCdk2_CycErem, Degradation_XicCdk2_CycErem).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Xicrem} = v_{11} + v_{12} - v_{25} \tag{118}$$

9.14 Species Cyc_total

Name Cyc_total

Initial concentration $1\ \mathrm{mmol} \cdot \mathrm{ml}^{-1}$

Involved in rule Cyc_total

One rule determines the species' quantity.

9.15 Species Xic_total

Name Xic_total

Initial concentration $0.999999999999993\ \mathrm{mmol} \cdot \mathrm{ml}^{-1}$

Involved in rule Xic_total

One rule determines the species' quantity.

9.16 Species Kin_a

Name Kin_a

Initial concentration $0.6\ \mathrm{mmol} \cdot \mathrm{ml}^{-1}$

This species takes part in two reactions (as a product in Kinase__regulation and as a modifier in Wee1_regulation).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Kin\_a} = v_{18} \tag{119}$$

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.

[a]Center for Bioinformatics Tübingen (ZBIT), Germany
[b]California Institute of Technology, Beckman Institute BNMC, Pasadena, United States
[c]European Bioinformatics Institute, Wellcome Trust Genome Campus, Hinxton, United Kingdom
[d]EML Research gGmbH, Heidelberg, Germany