SBML Model Report

Model name: "Sriram2007_CellCycle"



May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 3 format. This model was created by Harish Dharuri¹ at August twelveth 2008 at 9:04 p.m. and last time modified at May 27th 2014 at 10:47 p.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 | 6 |
| events | 0 | constraints | 0 |
| reactions | 18 | function definitions | 0 |
| global parameters | 25 | unit definitions | 5 |
| rules | 0 | initial assignments | 0 |

Model Notes

The model reproduces the time profile of species depicted in Figure 12a and 12 b. The authors communicated to the curator that there is a typo in the paper, the values of kd1 and kd2 are reversed. Model successfully reproduced using MathSBML.

2 Unit Definitions

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

 $^{{}^{1}}California\ Institute\ of\ Technology,\ {\tt hdharuri@cds.caltech.edu}$

2.1 Unit substance

Name nano mole

Definition nmol

2.2 Unit time

Name minutes

Definition 60 s

2.3 Unit nM_min_1

Name nM_min_1

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

2.4 Unit nM

Name nM

Definition $nmol \cdot l^{-1}$

2.5 Unit min_1

Name min_1

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

2.6 Unit volume

Notes Litre is the predefined SBML unit for volume.

Definition 1

2.7 Unit area

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

Definition m^2

2.8 Unit length

Notes Metre is the predefined SBML unit for length since SBML Level 2 Version 1.

Definition m

3 Compartment

This model contains one compartment.

Table 2: Properties of all compartments.

| Id | Name | SBO | Spatial Dimensions | Size | Unit | Constant | Outside |
|-------------|------|-----|--------------------|------|-------|----------|---------|
| compartment | | | 3 | 1 | litre | Ø | |

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 7 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 |
|----|------|-------------|-------------------------------------|----------|----------|
| | | | | | Condi- |
| | | | | | tion |
| T1 | T1 | compartment | $nmol \cdot l^{-1}$ | | |
| T2 | T2 | compartment | $\mathrm{nmol}\cdot\mathrm{l}^{-1}$ | \Box | \Box |
| T3 | Т3 | compartment | $\mathrm{nmol}\cdot\mathrm{l}^{-1}$ | \Box | \Box |
| C1 | C1 | compartment | $\mathrm{nmol}\cdot\mathrm{l}^{-1}$ | \Box | \Box |
| C2 | C2 | compartment | $nmol \cdot l^{-1}$ | | \Box |
| C3 | C3 | compartment | $nmol \cdot l^{-1}$ | | |

5 Parameters

This model contains 25 global parameters.

Table 4: Properties of each parameter.

| Id | Name | SBO | Value | Unit | Constant |
|------|------|-----|--------|---|---------------------------|
| | | | 0.900 | $nmol \cdot l^{-1} \cdot (60 \text{ s})^{-1}$ | |
| vd1 | | | 6.000 | $nmol \cdot 1^{-1} \cdot (60 \text{ s})^{-1}$ | |
| n | | | 2.000 | dimensionless | |
| km1 | | | 5.000 | $nmol \cdot l^{-1}$ | |
| kc1 | | | 0.200 | $(60 \text{ s})^{-1}$ | |
| kd1 | | | 0.800 | $(60 \text{ s})^{-1}$ | |
| j2 | | | 0.500 | $nmol \cdot l^{-1} \cdot (60 \text{ s})^{-1}$ | |
| vd2 | | | 1.052 | $n \text{mol} \cdot 1^{-1} \cdot (60 \text{ s})^{-1}$ | |
| km2 | | | 5.000 | $nmol \cdot l^{-1}$ | $\overline{\mathbf{Z}}$ |
| kc2 | | | 0.220 | $(60 \text{ s})^{-1}$ | |
| kd2 | | | 0.900 | $(60 \text{ s})^{-1}$ | |
| j3 | | | 0.200 | $nmol \cdot l^{-1} \cdot (60 \text{ s})^{-1}$ | |
| vd3 | | | 3.000 | $nmol \cdot l^{-1} \cdot (60 \text{ s})^{-1}$ | |
| km3 | | | 5.000 | $nmol \cdot l^{-1}$ | $\overline{\mathbf{Z}}$ |
| kc3 | | | 0.600 | $(60 \text{ s})^{-1}$ | |
| kd3 | | | 0.800 | $(60 \text{ s})^{-1}$ | |
| v12 | | | 15.000 | $nmol \cdot l^{-1} \cdot (60 \text{ s})^{-1}$ | |
| k120 | | | 10.000 | $nmol \cdot l^{-1}$ | $\overline{\mathbf{Z}}$ |
| kd4 | | | 0.160 | $(60 \text{ s})^{-1}$ | |
| v11 | | | 15.000 | $nmol \cdot l^{-1} \cdot (60 \text{ s})^{-1}$ | |
| k110 | | | 10.000 | $nmol \cdot l^{-1}$ | $\overline{\mathbf{Z}}$ |
| kd5 | | | 0.160 | $(60 \text{ s})^{-1}$ | $\overline{\mathbf{Z}}$ |
| v10 | | | 15.000 | $nmol \cdot l^{-1} \cdot (60 \text{ s})^{-1}$ | $\overline{\mathbf{Z}}$ |
| k100 | | | 10.000 | $nmol \cdot l^{-1}$ | $\overline{\mathbb{Z}}$ |
| kd6 | | | 0.160 | $(60 \text{ s})^{-1}$ | $ \overline{\mathbb{Z}} $ |

6 Reactions

This model contains 18 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

| N₀ | Id | Name | Reaction Equation | SBO |
|----|-----|------|---|-----|
| 1 | R1 | | $\emptyset \longrightarrow T1$ | |
| 2 | R2 | | $\emptyset \xrightarrow{\mathbf{T3}} \mathbf{T1}$ | |
| 3 | R3 | | $\emptyset \xrightarrow{\mathbf{C1}} \mathbf{T1}$ | |
| 4 | R4 | | $T1 \longrightarrow \emptyset$ | |
| 5 | R5 | | $\emptyset \longrightarrow T2$ | |
| 6 | R6 | | $\emptyset \xrightarrow{\mathrm{T1}} \mathrm{T2}$ | |
| 7 | R7 | | $\emptyset \xrightarrow{\mathbf{C2}} \mathbf{T2}$ | |
| 8 | R8 | | $T2 \longrightarrow \emptyset$ | |
| 9 | R9 | | $\emptyset \longrightarrow T3$ | |
| 10 | R10 | | $\emptyset \xrightarrow{\mathrm{T2}} \mathrm{T3}$ | |
| 11 | R11 | | $\emptyset \xrightarrow{\mathbf{C3}} \mathbf{T3}$ | |
| 12 | R12 | | $T3 \longrightarrow \emptyset$ | |
| 13 | R13 | | $\emptyset \xrightarrow{\text{T1, C2}} \text{C1}$ | |
| 14 | R14 | | $C1 \longrightarrow \emptyset$ | |
| 15 | R15 | | $\emptyset \xrightarrow{\text{T2, C3}} \text{C2}$ | |
| 16 | R16 | | $C2 \longrightarrow \emptyset$ | |
| 17 | R17 | | $\emptyset \xrightarrow{\text{T3, C1}} \text{C3}$ | |
| 18 | R18 | | $C3 \longrightarrow \emptyset$ | |

6.1 Reaction R1

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

Reaction equation

$$\emptyset \longrightarrow T1$$
 (1)

Product

Table 6: Properties of each product.

| Id | Name | SBO |
|----|------|-----|
| T1 | T1 | |

Kinetic Law

 $\textbf{Derived unit} \ \operatorname{nmol} \cdot \left(60 \ s\right)^{-1}$

$$v_1 = \text{vol}(\text{compartment}) \cdot \text{j1}$$
 (2)

6.2 Reaction R2

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

Reaction equation

$$\emptyset \xrightarrow{T3} T1 \tag{3}$$

Modifier

Table 7: Properties of each modifier.

| Id | Name | SBO |
|----|------|-----|
| Т3 | T3 | |

Table 8: Properties of each product.

| Id | Name | SBO |
|----|------|-----|
| T1 | T1 | |

Derived unit $1.000000000000038 \cdot 10^{-9} \text{ mol} \cdot (60 \text{ s})^{-1}$

$$v_2 = \frac{\text{vol (compartment)} \cdot \text{vd1} \cdot [\text{T3}]^n}{\text{km1}^n + [\text{T3}]^n}$$
(4)

6.3 Reaction R3

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

Reaction equation

$$\emptyset \xrightarrow{C1} T1 \tag{5}$$

Modifier

Table 9: Properties of each modifier.

| Id | Name | SBO |
|----|------|-----|
| C1 | C1 | |

Product

Table 10: Properties of each product.

| Id | Name | SBO |
|----|------|-----|
| T1 | T1 | |

Kinetic Law

Derived unit $(60 \text{ s})^{-1} \cdot \text{nmol}$

$$v_3 = \text{vol}(\text{compartment}) \cdot \text{kc1} \cdot [\text{C1}]$$
 (6)

6.4 Reaction R4

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

Reaction equation

$$T1 \longrightarrow \emptyset$$
 (7)

Reactant

Table 11: Properties of each reactant.

| Id | Name | SBO |
|----|------|-----|
| T1 | T1 | |

Kinetic Law

Derived unit $(60 \text{ s})^{-1} \cdot \text{nmol}$

$$v_4 = \text{vol}\left(\text{compartment}\right) \cdot \text{kd1} \cdot [\text{T1}]$$
 (8)

6.5 Reaction R5

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

Reaction equation

$$\emptyset \longrightarrow T2$$
 (9)

Product

Table 12: Properties of each product.

| Id | Name | SBO |
|----|------|-----|
| T2 | T2 | |

Kinetic Law

Derived unit $nmol \cdot (60 \text{ s})^{-1}$

$$v_5 = \text{vol}(\text{compartment}) \cdot \text{j2}$$
 (10)

6.6 Reaction R6

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

Reaction equation

$$\emptyset \xrightarrow{T1} T2 \tag{11}$$

Modifier

Table 13: Properties of each modifier.

| Id | Name | SBO |
|----|------|-----|
| T1 | T1 | |

Product

Table 14: Properties of each product.

| Id | Name | SBO |
|----|------|-----|
| T2 | T2 | |

Kinetic Law

 $\textbf{Derived unit} \ \ 1.000000000000038 \cdot 10^{-9} \ mol \cdot (60 \ s)^{-1}$

$$v_6 = \frac{\text{vol (compartment)} \cdot \text{vd2} \cdot [\text{T1}]^n}{\text{km2}^n + [\text{T1}]^n}$$
 (12)

6.7 Reaction R7

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

Reaction equation

$$\emptyset \xrightarrow{C2} T2 \tag{13}$$

Modifier

Table 15: Properties of each modifier.

| Id | Name | SBO |
|----|------|-----|
| C2 | C2 | |

Table 16: Properties of each product.

| Id | Name | SBO |
|----|------|-----|
| T2 | T2 | |

Derived unit $(60 \text{ s})^{-1} \cdot \text{nmol}$

$$v_7 = \text{vol}\left(\text{compartment}\right) \cdot \text{kc2} \cdot [\text{C2}]$$
 (14)

6.8 Reaction R8

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

Reaction equation

$$T2 \longrightarrow \emptyset$$
 (15)

Reactant

Table 17: Properties of each reactant.

| Id | Name | SBO |
|----|------|-----|
| T2 | T2 | |

Kinetic Law

Derived unit $(60 \text{ s})^{-1} \cdot \text{nmol}$

$$v_8 = \text{vol} \left(\text{compartment} \right) \cdot \text{kd2} \cdot [\text{T2}]$$
 (16)

6.9 Reaction R9

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

Reaction equation

$$\emptyset \longrightarrow T3$$
 (17)

Table 18: Properties of each product.

| Id | Name | SBO |
|----|------|-----|
| Т3 | T3 | |

 $\textbf{Derived unit} \ \operatorname{nmol} \cdot \left(60 \ s\right)^{-1}$

$$v_9 = \text{vol}(\text{compartment}) \cdot \text{j3}$$
 (18)

6.10 Reaction R10

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

Reaction equation

$$\emptyset \xrightarrow{T2} T3 \tag{19}$$

Modifier

Table 19: Properties of each modifier.

| Id | Name | SBO |
|----|------|-----|
| T2 | T2 | |

Product

Table 20: Properties of each product.

| Id | Name | SBO |
|----|------|-----|
| Т3 | T3 | |

Kinetic Law

 $\textbf{Derived unit} \ \ 1.000000000000038 \cdot 10^{-9} \ mol \cdot (60 \ s)^{-1}$

$$v_{10} = \frac{\text{vol}\left(\text{compartment}\right) \cdot \text{vd3} \cdot [\text{T2}]^{\text{n}}}{\text{km3}^{\text{n}} + [\text{T2}]^{\text{n}}}$$
(20)

6.11 Reaction R11

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

Reaction equation

$$\emptyset \xrightarrow{C3} T3 \tag{21}$$

Modifier

Table 21: Properties of each modifier.

| Id | Name | SBO |
|----|------|-----|
| СЗ | C3 | |

Product

Table 22: Properties of each product.

| Id | Name | SBO |
|----|------|-----|
| Т3 | Т3 | |

Kinetic Law

Derived unit $(60 \text{ s})^{-1} \cdot \text{nmol}$

$$v_{11} = \text{vol}\left(\text{compartment}\right) \cdot \text{kc3} \cdot [\text{C3}]$$
 (22)

6.12 Reaction R12

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

Reaction equation

$$T3 \longrightarrow \emptyset$$
 (23)

Reactant

Table 23: Properties of each reactant.

| Id | Name | SBO |
|----|------|-----|
| Т3 | T3 | |

Kinetic Law

Derived unit $(60 \text{ s})^{-1} \cdot \text{nmol}$

$$v_{12} = \text{vol} \left(\text{compartment} \right) \cdot \text{kd3} \cdot [\text{T3}]$$
 (24)

6.13 Reaction R13

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

Reaction equation

$$\emptyset \xrightarrow{\text{T1, C2}} \text{C1} \tag{25}$$

Modifiers

Table 24: Properties of each modifier.

| Id | Name | SBO |
|----|------|-----|
| T1 | T1 | |
| C2 | C2 | |

Product

Table 25: Properties of each product.

| Id | Name | SBO |
|----|------|-----|
| C1 | C1 | |

Kinetic Law

Derived unit $1.000000000000038 \cdot 10^{-9} \text{ mol} \cdot (60 \text{ s})^{-1}$

$$v_{13} = \frac{\text{vol (compartment)} \cdot \text{v12} \cdot [\text{T1}]^{\text{n}}}{\text{k120}^{\text{n}} + [\text{T1}]^{\text{n}} + [\text{C2}]^{\text{n}}}$$
 (26)

6.14 Reaction R14

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

Reaction equation

$$C1 \longrightarrow \emptyset$$
 (27)

Reactant

Table 26: Properties of each reactant.

| Id | Name | SBO |
|----|------|-----|
| C1 | C1 | |

Derived unit $(60 \text{ s})^{-1} \cdot \text{nmol}$

$$v_{14} = \text{vol}\left(\text{compartment}\right) \cdot \text{kd4} \cdot [\text{C1}]$$
 (28)

6.15 Reaction R15

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

Reaction equation

$$\emptyset \xrightarrow{\text{T2, C3}} \text{C2} \tag{29}$$

Modifiers

Table 27: Properties of each modifier.

| Id | Name | SBO |
|----|------|-----|
| T2 | T2 | |
| C3 | C3 | |

Product

Table 28: Properties of each product.

| Id | Name | SBO |
|----|------|-----|
| C2 | C2 | |

Kinetic Law

Derived unit $1.000000000000038 \cdot 10^{-9} \text{ mol} \cdot (60 \text{ s})^{-1}$

$$v_{15} = \frac{\text{vol (compartment)} \cdot \text{v11} \cdot [\text{T2}]^n}{\text{k110}^n + [\text{T2}]^n + [\text{C3}]^n}$$
(30)

6.16 Reaction R16

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

Reaction equation

$$C2 \longrightarrow \emptyset$$
 (31)

Reactant

Table 29: Properties of each reactant.

| Id | Name | SBO |
|----|------|-----|
| C2 | C2 | |

Kinetic Law

Derived unit $(60 \text{ s})^{-1} \cdot \text{nmol}$

$$v_{16} = \text{vol}\left(\text{compartment}\right) \cdot \text{kd5} \cdot [\text{C2}]$$
 (32)

6.17 Reaction R17

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

Reaction equation

$$\emptyset \xrightarrow{\text{T3, C1}} \text{C3} \tag{33}$$

Modifiers

Table 30: Properties of each modifier.

| | • | |
|----|------|-----|
| Id | Name | SBO |
| Т3 | Т3 | |
| C1 | C1 | |
| | | |

Table 31: Properties of each product.

| Id | Name | SBO |
|----|------|-----|
| СЗ | C3 | |

Derived unit $1.000000000000038 \cdot 10^{-9} \text{ mol} \cdot (60 \text{ s})^{-1}$

$$v_{17} = \frac{\text{vol (compartment)} \cdot \text{v10} \cdot [\text{T3}]^{\text{n}}}{\text{k100}^{\text{n}} + [\text{T3}]^{\text{n}} + [\text{C1}]^{\text{n}}}$$
(34)

6.18 Reaction R18

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

Reaction equation

$$C3 \longrightarrow \emptyset$$
 (35)

Reactant

Table 32: Properties of each reactant.

| Id | Name | SBO |
|----|------|-----|
| СЗ | C3 | |

Kinetic Law

Derived unit $(60 \text{ s})^{-1} \cdot \text{nmol}$

$$v_{18} = \text{vol} (\text{compartment}) \cdot \text{kd6} \cdot [\text{C3}]$$
 (36)

7 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.

7.1 Species T1

Name T1

Initial concentration 6 nmol·l⁻¹

This species takes part in six reactions (as a reactant in R4 and as a product in R1, R2, R3 and as a modifier in R6, R13).

$$\frac{d}{dt}T1 = v_1 + v_2 + v_3 - v_4 \tag{37}$$

7.2 Species T2

Name T2

Initial concentration $5 \text{ nmol} \cdot l^{-1}$

This species takes part in six reactions (as a reactant in R8 and as a product in R5, R6, R7 and as a modifier in R10, R15).

$$\frac{d}{dt}T2 = v_5 + v_6 + v_7 - v_8 \tag{38}$$

7.3 Species T3

Name T3

Initial concentration 1 nmol·l⁻¹

This species takes part in six reactions (as a reactant in R12 and as a product in R9, R10, R11 and as a modifier in R2, R17).

$$\frac{\mathrm{d}}{\mathrm{d}t}T3 = v_9 + v_{10} + v_{11} - v_{12} \tag{39}$$

7.4 Species C1

Name C1

Initial concentration $0 \text{ nmol} \cdot 1^{-1}$

This species takes part in four reactions (as a reactant in R14 and as a product in R13 and as a modifier in R3, R17).

$$\frac{d}{dt}C1 = v_{13} - v_{14} \tag{40}$$

7.5 Species C2

Name C2

Initial concentration $0 \text{ nmol} \cdot 1^{-1}$

This species takes part in four reactions (as a reactant in R16 and as a product in R15 and as a modifier in R7, R13).

$$\frac{d}{dt}C2 = v_{15} - v_{16} \tag{41}$$

7.6 Species C3

Name C3

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

This species takes part in four reactions (as a reactant in R18 and as a product in R17 and as a modifier in R11, R15).

$$\frac{d}{dt}C3 = v_{17} - v_{18} \tag{42}$$

 $\mathfrak{BML2}^{lAT}$ EX 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.

^aCenter for Bioinformatics Tübingen (ZBIT), Germany

^bCalifornia Institute of Technology, Beckman Institute BNMC, Pasadena, United States

^cEuropean Bioinformatics Institute, Wellcome Trust Genome Campus, Hinxton, United Kingdom

^dEML Research gGmbH, Heidelberg, Germany