SBML Model Report

Model name: "Ibrahim2008_MCC_assembly_model_KDM"

May 5, 2016

1 General Overview

This is a document in SBML Level 2 Version 3 format. This model was created by the following five authors: Lukas Endler[1], Eberhard Schmitt[2], Peter Dittrich[3], Stephan Diekmann[4] and Bashar Ibrahim[5] at November 27th 2008 at 10:56 a. m. and last time modified at September 23rd 2009 at 5:12 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	8
events	1	constraints	0
reactions	6	function definitions	0
global parameters	12	unit definitions	2
rules	0	initial assignments	0

Model Notes

BioSystems (2007), doi:10.1016/j.biosystems.2008.06.007

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***In-silico* study of kinetochore control, amplification, and inhibition effects in MCC assembly**

Bashar Ibrahim, Eberhard Schmitt, Peter Dittrich, Stephan Diekmann

This is the kinetochore dependent MCC model (KDM) from the article. For the kinetochore independent MCC model (KIM) replace *u*k4f* in *R4* by *k4f* and *u*k5f* in *R5* by *k5f* .

2 Unit Definitions

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

2.1 Unit ps

Name per second

Definition s^{-1}

2.2 Unit pMps

Name liter per mole per second

Definition $l \cdot mol^{-1} \cdot s^{-1}$

2.3 Unit substance

Notes Mole is the predefined SBML unit for `substance`.

Definition mol

2.4 Unit volume

Notes Litre is the predefined SBML unit for `volume`.

Definition l

2.5 Unit area

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

Definition m^2

2.6 Unit length

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

Definition m

2.7 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
Cytoplasm	Cytoplasm		3	1	litre	☑	

3.1 Compartment Cytoplasm

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

Name Cytoplasm

4 Species

This model contains eight 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
Mad1_CMad2	Mad1:C-Mad2	Cytoplasm	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
OMad2	O-Mad2	Cytoplasm	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Mad1_CMad2_OMad2	Mad1:C-Mad2:O-Mad2*	Cytoplasm	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Cdc20	Cdc20	Cytoplasm	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Cdc20_CMad2	Cdc20:C-Mad2	Cytoplasm	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Bub3_BubR1	Bub3:BubR1	Cytoplasm	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
MCC	MCC	Cytoplasm	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Bub3_BubR1_Cdc20	Bub3:BubR1:Cdc20	Cytoplasm	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟

5 Parameters

This model contains twelve global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k3f		0000338	0.010	s^{-1}	☑
kf6		0000339	1000.000	$l \cdot mol^{-1} \cdot s^{-1}$	☑
k5f		0000339	10000.000	$l \cdot mol^{-1} \cdot s^{-1}$	☑
k5r		0000038	0.200	s^{-1}	☑
k2f		0000339	10^7	$l \cdot mol^{-1} \cdot s^{-1}$	☑
k1f		0000339	200000.000	$l \cdot mol^{-1} \cdot s^{-1}$	☑
k1r		0000338	0.200	s^{-1}	☑
k4f		0000339	10^7	$l \cdot mol^{-1} \cdot s^{-1}$	☑
k4r		0000338	0.020	s^{-1}	☑
u			1.000	dimensionless	☐
const_val_0			0.000	dimensionless	☑
const_val_1			1.000	dimensionless	☑

6 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.

6.1 Event mt_attachment

Name Microtubule attachment

Trigger condition

$$\text{time} > 2000 \tag{1}$$

Assignment

$$\text{u} = \text{const\_val\_0} \tag{2}$$

7 Reactions

This model contains six reactions. All reactions are listed in the following table and are subsequently described in detail. If a reaction is affected by a modifier, the identifier of this species is written above the reaction arrow.

Table 5: Overview of all reactions

№	Id	Name	Reaction Equation	SBO
1	R1		$\text{Mad1\_CMad2} + \text{OMad2} \rightleftharpoons \text{Mad1\_CMad2\_OMad2}$	0000177
2	R2		$\text{Mad1\_CMad2\_OMad2} + \text{Cdc20} \longrightarrow \text{Mad1\_CMad2} + \text{Cdc20\_CMad2}$	0000176
3	R3		$\text{Cdc20\_CMad2} \longrightarrow \text{Cdc20} + \text{OMad2}$	0000180
4	R4		$\text{Cdc20\_CMad2} + \text{Bub3\_BubR1} \rightleftharpoons \text{MCC}$	0000177
5	R5		$\text{Bub3\_BubR1} + \text{Cdc20} \rightleftharpoons \text{Bub3\_BubR1\_Cdc20}$	0000177
6	R6		$\text{OMad2} + \text{Cdc20} \longrightarrow \text{Cdc20\_CMad2}$	0000177

7.1 Reaction R1

This is a reversible reaction of two reactants forming one product.

SBO:0000177 non-covalent binding

Reaction equation

$$\text{Mad1\_CMad2} + \text{OMad2} \rightleftharpoons \text{Mad1\_CMad2\_OMad2} \tag{3}$$

Reactants

Table 6: Properties of each reactant.

Id	Name	SBO
Mad1_CMad2	Mad1:C-Mad2	0000336
OMad2	O-Mad2	0000336

Product

Table 7: Properties of each product.

Id	Name	SBO
Mad1_CMad2_OMad2	Mad1:C-Mad2:O-Mad2*	0000011

Kinetic Law

SBO:0000101 mass action rate law for second order forward, first order reverse, reversible reactions, two reactants, continuous scheme

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

$$v_1 = \mathrm{vol}\,(\mathrm{Cytoplasm}) \cdot (\mathrm{u} \cdot \mathrm{k1f} \cdot [\mathrm{Mad1\_CMad2}] \cdot [\mathrm{OMad2}] - \mathrm{k1r} \cdot [\mathrm{Mad1\_CMad2\_OMad2}]) \tag{4}$$

7.2 Reaction R2

This is an irreversible reaction of two reactants forming two products.

SBO:0000176 biochemical reaction

Reaction equation

$$\text{Mad1\_CMad2\_OMad2} + \text{Cdc20} \longrightarrow \text{Mad1\_CMad2} + \text{Cdc20\_CMad2} \tag{5}$$

Reactants

Table 8: Properties of each reactant.

Id	Name	SBO
Mad1_CMad2_OMad2	Mad1:C-Mad2:O-Mad2*	0000336
Cdc20	Cdc20	0000336

Products

Table 9: Properties of each product.

Id	Name	SBO
Mad1_CMad2	Mad1:C-Mad2	0000011
Cdc20_CMad2	Cdc20:C-Mad2	0000011

Kinetic Law

SBO:0000054 mass action rate law for second order irreversible reactions, two reactants, continuous scheme

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

$$v_2 = \mathrm{vol}\,(\mathrm{Cytoplasm}) \cdot \mathrm{u} \cdot \mathrm{k2f} \cdot [\mathrm{Mad1\_CMad2\_OMad2}] \cdot [\mathrm{Cdc20}] \tag{6}$$

7.3 Reaction R3

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

SBO:0000180 dissociation

Reaction equation

$$\mathrm{Cdc20\_CMad2} \longrightarrow \mathrm{Cdc20} + \mathrm{OMad2} \tag{7}$$

Reactant

Table 10: Properties of each reactant.

Id	Name	SBO
Cdc20_CMad2	Cdc20:C-Mad2	0000010

Products

Table 11: Properties of each product.

Id	Name	SBO
Cdc20	Cdc20	0000011
OMad2	O-Mad2	0000011

Kinetic Law

SBO:0000049 mass action rate law for first order irreversible reactions, continuous scheme

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

$$v_3 = \text{vol}(\text{Cytoplasm}) \cdot \text{k3f} \cdot [\text{Cdc20\_CMad2}] \tag{8}$$

7.4 Reaction R4

This is a reversible reaction of two reactants forming one product.

SBO:0000177 non-covalent binding

Reaction equation

$$\text{Cdc20\_CMad2} + \text{Bub3\_BubR1} \rightleftharpoons \text{MCC} \tag{9}$$

Reactants

Table 12: Properties of each reactant.

Id	Name	SBO
Cdc20_CMad2	Cdc20:C-Mad2	0000336
Bub3_BubR1	Bub3:BubR1	0000336

Product

Table 13: Properties of each product.

Id	Name	SBO
MCC	MCC	0000011

Kinetic Law

SBO:0000103 mass action rate law for second order forward, second order reverse, reversible reactions, two reactants, one product, continuous scheme

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

$$v_4 = \text{vol}(\text{Cytoplasm}) \cdot (\text{u} \cdot \text{k4f} \cdot [\text{Cdc20\_CMad2}] \cdot [\text{Bub3\_BubR1}] - \text{k4r} \cdot [\text{MCC}]) \quad (10)$$

7.5 Reaction R5

This is a reversible reaction of two reactants forming one product.

SBO:0000177 non-covalent binding

Reaction equation

$$\text{Bub3\_BubR1} + \text{Cdc20} \rightleftharpoons \text{Bub3\_BubR1\_Cdc20} \quad (11)$$

Reactants

Table 14: Properties of each reactant.

Id	Name	SBO
Bub3_BubR1	Bub3:BubR1	0000336
Cdc20	Cdc20	0000336

Product

Table 15: Properties of each product.

Id	Name	SBO
Bub3_BubR1_Cdc20	Bub3:BubR1:Cdc20	0000011

Kinetic Law

SBO:0000103 mass action rate law for second order forward, second order reverse, reversible reactions, two reactants, one product, continuous scheme

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

$$v_5 = \text{vol}(\text{Cytoplasm}) \cdot (\text{u} \cdot \text{k5f} \cdot [\text{Bub3\_BubR1}] \cdot [\text{Cdc20}] - \text{k5r} \cdot [\text{Bub3\_BubR1\_Cdc20}]) \quad (12)$$

7.6 Reaction R6

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

SBO:0000177 non-covalent binding

Reaction equation

$$\mathrm{OMad2} + \mathrm{Cdc20} \longrightarrow \mathrm{Cdc20\_CMad2} \tag{13}$$

Reactants

Table 16: Properties of each reactant.

Id	Name	SBO
OMad2	O-Mad2	0000336
Cdc20	Cdc20	0000336

Product

Table 17: Properties of each product.

Id	Name	SBO
Cdc20_CMad2	Cdc20:C-Mad2	0000011

Kinetic Law

SBO:0000054 mass action rate law for second order irreversible reactions, two reactants, continuous scheme

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

$$v_6 = \mathrm{vol}\,(\mathrm{Cytoplasm}) \cdot \mathrm{kf6} \cdot [\mathrm{OMad2}] \cdot [\mathrm{Cdc20}] \tag{14}$$

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.

8.1 Species Mad1_CMad2

Name Mad1:C-Mad2

SBO:0000297 protein complex

Initial concentration $5 \cdot 10^{-8}\ \mathrm{mol} \cdot \mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in R1 and as a product in R2).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Mad1\_CMad2} = v_2 - v_1 \tag{15}$$

8.2 Species OMad2

Name O-Mad2

Notes Open conformation of Mad2

Initial concentration $1.3 \cdot 10^{-7}$ mol $\cdot$ l^{-1}

This species takes part in three reactions (as a reactant in R1, R6 and as a product in R3).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{OMad2} = v_3 - v_1 - v_6 \tag{16}$$

8.3 Species Mad1_CMad2_OMad2

Name Mad1:C-Mad2:O-Mad2*

SBO:0000297 protein complex

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

This species takes part in two reactions (as a reactant in R2 and as a product in R1).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Mad1\_CMad2\_OMad2} = v_1 - v_2 \tag{17}$$

8.4 Species Cdc20

Name Cdc20

Initial concentration $2.2 \cdot 10^{-7}$ mol $\cdot$ l^{-1}

This species takes part in four reactions (as a reactant in R2, R5, R6 and as a product in R3).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Cdc20} = v_3 - v_2 - v_5 - v_6 \tag{18}$$

8.5 Species Cdc20_CMad2

Name Cdc20:C-Mad2

SBO:0000297 protein complex

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

This species takes part in four reactions (as a reactant in R3, R4 and as a product in R2, R6).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Cdc20\_CMad2} = v_2 + v_6 - v_3 - v_4 \tag{19}$$

8.6 Species Bub3_BubR1

Name Bub3:BubR1

SBO:0000297 protein complex

Initial concentration $1.3 \cdot 10^{-7}$ mol $\cdot$ l^{-1}

This species takes part in two reactions (as a reactant in R4, R5).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Bub3\_BubR1} = -v_4 - v_5 \tag{20}$$

8.7 Species MCC

Name MCC

SBO:0000297 protein complex

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

This species takes part in one reaction (as a product in R4).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{MCC} = v_4 \tag{21}$$

8.8 Species Bub3_BubR1_Cdc20

Name Bub3:BubR1:Cdc20

SBO:0000297 protein complex

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

This species takes part in one reaction (as a product in R5).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Bub3\_BubR1\_Cdc20} = v_5 \tag{22}$$

A Glossary of Systems Biology Ontology Terms

SBO:0000010 reactant: Substance consumed by a chemical reaction. Reactants react with each other to form the products of a chemical reaction. In a chemical equation the Reactants are the elements or compounds on the left hand side of the reaction equation. A reactant can be consumed and produced by the same reaction, its global quantity remaining unchanged

SBO:0000011 product: Substance that is produced in a reaction. In a chemical equation the Products are the elements or compounds on the right hand side of the reaction equation. A product can be produced and consumed by the same reaction, its global quantity remaining unchanged

SBO:0000038 reverse unimolecular rate constant, continuous case: Numerical parameter that quantifies the reverse velocity of a chemical reaction involving only one product. This parameter encompasses all the contributions to the velocity except the quantity of the product. It is to be used in a reaction modelled using a continuous framework

SBO:0000049 mass action rate law for first order irreversible reactions, continuous scheme: Reaction scheme where the products are created from the reactants and the change of a product quantity is proportional to the product of reactant activities. The reaction scheme does not include any reverse process that creates the reactants from the products. The change of a product quantity is proportional to the quantity of one reactant. It is to be used in a reaction modelled using a continuous framework.

SBO:0000054 mass action rate law for second order irreversible reactions, two reactants, continuous scheme: Reaction scheme where the products are created from the reactants and the change of a product quantity is proportional to the product of reactant activities. The reaction scheme does not include any reverse process that creates the reactants from the products. The change of a product quantity is proportional to the product of two reactant quantities. It is to be used in a reaction modelled using a continuous framework.

SBO:0000101 mass action rate law for second order forward, first order reverse, reversible reactions, two reactants, continuous scheme: Reaction scheme where the products are created from the reactants and the change of a product quantity is proportional to the product of reactant activities. The reaction scheme does include a reverse process that creates the reactants from the products. The rate of the forward process is proportional to the product of two reactant quantities. The rate of the reverse process is proportional to the quantity of one product. It is to be used in a reaction modelled using a continuous framework.

SBO:0000103 mass action rate law for second order forward, second order reverse, reversible reactions, two reactants, one product, continuous scheme: Reaction scheme where the products are created from the reactants and the change of a product quantity is proportional to the product of reactant activities. The reaction scheme does include a reverse process that creates the reactants from the products. The rate of the forward process is proportional to the product of two reactant quantities. The rate of the reverse process is proportional to the square of one product quantity. It is to be used in a reaction modelled using a continuous framework.

SBO:0000176 biochemical reaction: An event involving one or more chemical entities that modifies the electrochemical structure of at least one of the participants.

SBO:0000177 non-covalent binding: Interaction between several biochemical entities that results in the formation of a non-covalent comple

SBO:0000180 dissociation: Transformation of a non-covalent complex that results in the formation of several independent biochemical entitie

SBO:0000297 protein complex: Macromolecular complex containing one or more polypeptide chains possibly associated with simple chemicals. CHEBI:3608

SBO:0000336 interactor: Entity participating in a physical or functional interaction

SBO:0000338 dissociation rate constant: Rate with which a complex dissociates into its components

SBO:0000339 bimolecular association rate constant: Rate with which two components associate into a complex

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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