SBML Model Report

Model name: “Suh2004_KCNQ_Regulation”

May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 1 format. This model was created by Harish Dharuri[1] at November nineth 2006 at 6:25 p. m. and last time modified at July fifth 2012 at 4:29 p. m. Table 1 gives an overview of the quantities of all components of this model.

Table 1: Number of components in this model, which are described in the following sections.

Element	Quantity	Element	Quantity
compartment types	0	compartments	3
species types	0	species	23
events	2	constraints	0
reactions	15	function definitions	0
global parameters	12	unit definitions	13
rules	9	initial assignments	0

Model Notes

The model reproduces FIG 11A and FIG 11B of the paper. However, please note that FIG 11B is a plot of normalised amounts versus time. The „stoichiometry„ field has been used to convert fluxes from membrane species to volume species. The value of 0.0009967 is a product of (Surface to Volume_M*(1/Avagadro’s number)*1E21. 0.6 is the surface to volume ratio of the plasma membrane, 1E21 is required for a unit surface to volume ratio and the Avagadro’s number is present in the denominator to convert molecules to moles. The model was successfully tested using MathSBML and SBML ODESolver.

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All the kinetic laws have the unit items per second , which requires the one reaction taking place in the cytoplasm - IP3Phosphatase - to include an explicit conversion factor both in the kinetic law and the stoichiometry of IP3_C . The kinetic law is multiplied and the stoichiometry divided by the number of molecules per micro-mole. This conversion factor is only required for correct units and can be replaced by 1, if it should lead to numerical problems.

To cite BioModels Database, please use: Li C, Donizelli M, Rodriguez N, Dharuri H, Endler L, Chelliah V, Li L, He E, Henry A, Stefan MI, Snoep JL, Hucka M, Le Novre N, Laibe C (2010) BioModels Database: An enhanced, curated and annotated resource for published quantitative kinetic models. BMC Syst Biol., 4:92.

2 Unit Definitions

This is an overview of 17 unit definitions of which four are predefined by SBML and not mentioned in the model.

2.1 Unit micromole

Definition µmol

2.2 Unit substance

Name items

Definition item

2.3 Unit items_per_micromole

Definition $\text{item} \cdot \mu\text{mol}^{-1}$

2.4 Unit molecules

Definition item

2.5 Unit um2

Definition μm^2

2.6 Unit molecules_um_2_s_1

Definition $\mu m^{-2} \cdot s^{-1} \cdot item$

2.7 Unit molecules_um_2

Definition $\mu m^{-2} \cdot item$

2.8 Unit uM_s_1

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

2.9 Unit s_1

Definition s^{-1}

2.10 Unit um2_molecules_1_s_1

Definition $item^{-1} \cdot \mu m^2 \cdot s^{-1}$

2.11 Unit uM_1_s_1

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

2.12 Unit uM_um_s_1

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

2.13 Unit microMolar

Name microMolar

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

2.14 Unit volume

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

Definition l

2.15 Unit area

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

Definition m^2

2.16 Unit length

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

Definition m

2.17 Unit time

Notes Second is the predefined SBML unit for time.

Definition s

3 Compartments

This model contains three compartments.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
EX	Extracellular		3	1		☑	
M	Membrane		2	1	μm^2	☑	EX
Cytoplasm	Cytoplasm		3	1		☑	M

3.1 Compartment EX

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

Name Extracellular

3.2 Compartment M

This is a two dimensional compartment with a constant size of one μm^2, which is surrounded by EX (Extracellular).

Name Membrane

3.3 Compartment Cytoplasm

This is a three dimensional compartment with a constant size of one litre, which is surrounded by M (Membrane).

Name Cytoplasm

4 Species

This model contains 23 species. The boundary condition of one of these species is set to `true` so that this 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
GTPgS_C	GTPgS_C	Cytoplasm	$\mu mol \cdot l^{-1}$	⊟	⊟
KCNQsites_M	KCNQsites_M	M	$item \cdot \mu m^{-2}$	⊟	⊟
PIP2_M	PIP2_M	M	$item \cdot \mu m^{-2}$	⊟	⊟
GGDPbS_M	GGDPbS_M	M	$item \cdot \mu m^{-2}$	⊟	⊟
Mg2_C	Mg2_C	Cytoplasm	$\mu mol \cdot l^{-1}$	⊟	☑
ATP_C	ATP_C	Cytoplasm	$\mu mol \cdot l^{-1}$	⊟	⊟
oxoM_EX	oxoM_EX	EX	$\mu mol \cdot l^{-1}$	⊟	⊟
GDPbS_C	GDPbS_C	Cytoplasm	$\mu mol \cdot l^{-1}$	⊟	⊟
GGTPMg_M	GGTPMg_M	M	$item \cdot \mu m^{-2}$	⊟	⊟
GDP_C	GDP_C	Cytoplasm	$\mu mol \cdot l^{-1}$	⊟	⊟
GTP_C	GTP_C	Cytoplasm	$\mu mol \cdot l^{-1}$	⊟	⊟
GGDPAlF4Mg_M	GGDPAIF4Mg_M	M	$item \cdot \mu m^{-2}$	⊟	⊟
ip3_C	IP3_C	Cytoplasm	$\mu mol \cdot l^{-1}$	⊟	⊟
AlF4_C	AIF4_C	Cytoplasm	$\mu mol \cdot l^{-1}$	⊟	⊟
G_M	G_M	M	$item \cdot \mu m^{-2}$	⊟	⊟
GGTP_M	GGTP_M	M	$item \cdot \mu m^{-2}$	⊟	⊟
GGDPAlF4_M	GGDPAIF4_M	M	$item \cdot \mu m^{-2}$	⊟	⊟
GGTPgS_M	GGTPgS_M	M	$item \cdot \mu m^{-2}$	⊟	⊟
PI_M	PI_M	M	$item \cdot \mu m^{-2}$	⊟	⊟
PIP_M	PIP_M	M	$item \cdot \mu m^{-2}$	⊟	⊟
PIP2xKCNQ_M	PIP2xKCNQ_M	M	$item \cdot \mu m^{-2}$	⊟	⊟

Id	Name	Compartment	Derived Unit	Constant	Boundary Condition
GGTPgSMg_M	GGTPgSMg_M	M	$\mathrm{item} \cdot \mu\mathrm{m}^{-2}$	⊟	⊟
GGDP_M	GGDP_M	M	$\mathrm{item} \cdot \mu\mathrm{m}^{-2}$	⊟	⊟

5 Parameters

This model contains twelve global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
MgSat20	MgSat20		0.000	dimensionless	☐
ATPSat300	ATPSat300		0.000	dimensionless	☐
MgSat10	MgSat10		0.000	dimensionless	☐
OxoSat	OxoSat		0.000	dimensionless	☐
Gactive	Gactive		0.000	$\mu m^{-2} \cdot item$	☐
ATPSat1000	ATPSat1000		0.000	dimensionless	☐
KMgGTPase	KMgGTPase		10.000	$\mu mol \cdot l^{-1}$	☑
Koxom	Koxom		8.000	$\mu mol \cdot l^{-1}$	☑
I_KCNQ	I_KCNQ		0.000	dimensionless	☐
nHill			1.800	dimensionless	☑
fGactive	fGactive		0.000	dimensionless	☐
NA_micro	NA(micro)		$6.022 \cdot 10^{17}$	$item \cdot \mu mol^{-1}$	☑

6 Rules

This is an overview of nine rules.

6.1 Rule MgSat20

Rule MgSat20 is an assignment rule for parameter MgSat20:

$$\text{MgSat20} = 1 \cdot \frac{1}{1 + 20 \cdot \frac{1}{[\text{Mg2\_C}]}} \tag{1}$$

6.2 Rule ATPSat1000

Rule ATPSat1000 is an assignment rule for parameter ATPSat1000:

$$\text{ATPSat1000} = 1 \cdot \frac{1}{1 + 1000 \cdot \frac{1}{0.5 + [\text{ATP\_C}]}} \tag{2}$$

6.3 Rule MgSat10

Rule MgSat10 is an assignment rule for parameter MgSat10:

$$\text{MgSat10} = 0.2 + 0.8 \cdot 1 \cdot \frac{1}{1 + \text{KMgGTPase} \cdot \frac{1}{[\text{Mg2\_C}]}} \tag{3}$$

6.4 Rule OxoSat

Rule OxoSat is an assignment rule for parameter OxoSat:

$$\text{OxoSat} = 1 \cdot \frac{1}{1 + \text{Koxom} \cdot \frac{1}{1.0E-5+[\text{oxoM\_EX}]}} \tag{4}$$

6.5 Rule fGactive

Rule fGactive is an assignment rule for parameter fGactive:

$$\text{fGactive} = \frac{[\text{GGTPMg\_M}] + [\text{GGTPgSMg\_M}] + [\text{GGDPAlF4Mg\_M}]}{200} \tag{5}$$

6.6 Rule Gactive

Rule Gactive is an assignment rule for parameter Gactive:

$$\text{Gactive} = [\text{GGTPMg\_M}] + [\text{GGTPgSMg\_M}] + [\text{GGDPAlF4Mg\_M}] \tag{6}$$

Derived unit $\text{item} \cdot \mu\text{m}^{-2}$

6.7 Rule ATPSat300

Rule ATPSat300 is an assignment rule for parameter ATPSat300:

$$\text{ATPSat300} = 1 \cdot \frac{1}{1 + 300 \cdot \frac{1}{0.5+[\text{ATP\_C}]}} \tag{7}$$

6.8 Rule I_KCNQ

Rule I_KCNQ is an assignment rule for parameter I_KCNQ:

$$\text{I\_KCNQ} = 1.33 \cdot (0.025 \cdot [\text{PIP2xKCNQ\_M}])^{\text{nHill}} \tag{8}$$

6.9 Rule GTP_C

Rule GTP_C is an assignment rule for species GTP_C:

$$\text{GTP\_C} = 100 - 50 \cdot \exp((0.00833333333333333 \cdot (290 + \text{t}))) \tag{9}$$

7 Events

This is an overview of two events. 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.

7.1 Event event_0000001

Trigger condition

$$t \geq 3 \tag{10}$$

Assignment

$$\text{oxoM\_EX} = 10 \tag{11}$$

7.2 Event event_0000002

Trigger condition

$$t \geq 8 \tag{12}$$

Assignment

$$\text{oxoM\_EX} = 0 \tag{13}$$

8 Reactions

This model contains 15 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	PIP5kinase	PIP5kinase	$9.967 \cdot 10^{-4}$ATP_C + PIP_M $\rightleftharpoons$ PIP2_M	
2	IP3Phosphatase	IP3Phosphatase	$1.666111296 \cdot 10^{-18}$ip3_C $\rightleftharpoons \emptyset$	
3	PIP2binding	PIP2binding	KCNQsites_M + PIP2_M $\rightleftharpoons$ PIP2xKCNQ_M	
4	MgonGGTPgS	MgonGGTPgS	GGTPgS_M $\overset{\text{Mg2\_C}}{\rightleftharpoons}$ GGTPgSMg_M	
5	GGTPase	GGTPase	GGTPMg_M $\rightleftharpoons$ GGDP_M	
6	GTPon	GTPon	G_M $\overset{\text{GTP\_C}}{\rightleftharpoons}$ GGTP_M	
7	GTPgSon	GTPgSon	$9.967 \cdot 10^{-4}$GTPgS_C + G_M $\rightleftharpoons$ GGTPgS_M	
8	GDPbSon	GDPbSon	G_M + $9.967 \cdot 10^{-4}$GDPbS_C $\rightleftharpoons$ GGDPbS_M	
9	MgGTPon	MgGTPon	GGTP_M $\overset{\text{Mg2\_C}}{\rightleftharpoons}$ GGTPMg_M	
10	GDPdissoc	GDPdissoc	GGDP_M $\overset{\text{oxoM\_EX}}{\rightleftharpoons}$ $9.967 \cdot 10^{-4}$GDP_C + G_M	
11	PIP2_5Pase	PIP2_5Pase	PIP2_M $\rightleftharpoons$ PIP_M	
12	PLC	PLC	PIP2_M $\rightleftharpoons$ $9.967 \cdot 10^{-4}$ip3_C	
13	AlF4on	AlF4on	$9.967 \cdot 10^{-4}$AlF4_C + GGDP_M $\rightleftharpoons$ GGDPAlF4_M	+
14	PI4Kinase	PI4Kinase	$9.967 \cdot 10^{-4}$ATP_C + PI_M $\rightleftharpoons$ PIP_M	
15	MgonGDPAlF4	MgonGDPAlF4	GGDPAlF4_M $\overset{\text{Mg2\_C}}{\rightleftharpoons}$ GGDPAlF4Mg_M	

8.1 Reaction PIP5kinase

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

Name PIP5kinase

Reaction equation

$$9.967 \cdot 10^{-4} \text{ATP\_C} + \text{PIP\_M} \rightleftharpoons \text{PIP2\_M} \tag{14}$$

Reactants

Table 6: Properties of each reactant.

Id	Name	SBO
ATP_C	ATP_C	
PIP_M	PIP_M	

Product

Table 7: Properties of each product.

Id	Name	SBO
PIP2_M	PIP2_M	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = (0.2 + 0.8 \cdot \text{MgSat20}) \cdot \text{kPIP5Kinase} \cdot [\text{PIP\_M}] \cdot \text{ATPSat300} \tag{15}$$

Table 8: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
kPIP5Kinase			0.06	s^{-1}	☑

8.2 Reaction IP3Phosphatase

This is a reversible reaction of one reactant forming no product.

Name IP3Phosphatase

Reaction equation

$$1.666111296 \cdot 10^{-18} \text{ip3\_C} \rightleftharpoons \emptyset \tag{16}$$

Reactant

Table 9: Properties of each reactant.

Id	Name	SBO
ip3_C	IP3_C	

Kinetic Law

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

$$v_2 = [\text{ip3\_C}] \cdot \text{kIP3ase} \cdot \text{vol}\,(\text{Cytoplasm}) \cdot \text{NA\_micro} \tag{17}$$

Table 10: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
kIP3ase			0.3	s^{-1}	☑

8.3 Reaction PIP2binding

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

Name PIP2binding

Reaction equation

$$\text{KCNQsites\_M} + \text{PIP2\_M} \rightleftharpoons \text{PIP2xKCNQ\_M} \tag{18}$$

Reactants

Table 11: Properties of each reactant.

Id	Name	SBO
KCNQsites_M	KCNQsites_M	
PIP2_M	PIP2_M	

Product

Table 12: Properties of each product.

Id	Name	SBO
PIP2xKCNQ_M	PIP2xKCNQ_M	

Kinetic Law

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

$$v_3 = (\mathrm{kPIP2on} \cdot [\mathrm{KCNQsites\_M}] \cdot [\mathrm{PIP2\_M}] + ((\mathrm{kPIP2off} \cdot [\mathrm{PIP2xKCNQ\_M}]))) \cdot \mathrm{area}(\mathrm{M}) \quad (19)$$

Table 13: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
kPIP2on			$2.5 \cdot 10^{-4}$	$\mathrm{item}^{-1} \cdot \mu\mathrm{m}^2 \cdot \mathrm{s}^{-1}$	☑
kPIP2off			0.250	s^{-1}	☑

8.4 Reaction MgonGGTPgS

This is a reversible reaction of one reactant forming one product influenced by one modifier.

Name MgonGGTPgS

Reaction equation

$$\mathrm{GGTPgS\_M} \overset{\mathrm{Mg2\_C}}{\rightleftharpoons} \mathrm{GGTPgSMg\_M} \quad (20)$$

Reactant

Table 14: Properties of each reactant.

Id	Name	SBO
GGTPgS_M	GGTPgS_M	

Modifier

Table 15: Properties of each modifier.

Id	Name	SBO
Mg2_C	Mg2_C	

Product

Table 16: Properties of each product.

Id	Name	SBO
GGTPgSMg_M	GGTPgSMg_M	

Kinetic Law

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

$$v_4 = \mathrm{kMg2onGTPgS} \cdot [\mathrm{GGTPgS\_M}] \cdot [\mathrm{Mg2\_C}] \cdot \mathrm{area}\,(\mathrm{M}) \tag{21}$$

Table 17: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
kMg2onGTPgS			0.002	$1 \cdot \mu\mathrm{mol}^{-1} \cdot \mathrm{s}^{-1}$	☑

8.5 Reaction GGTPase

This is a reversible reaction of one reactant forming one product.

Name GGTPase

Reaction equation

$$\mathrm{GGTPMg\_M} \rightleftharpoons \mathrm{GGDP\_M} \tag{22}$$

Reactant

Table 18: Properties of each reactant.

Id	Name	SBO
GGTPMg_M	GGTPMg_M	

Product

Table 19: Properties of each product.

Id	Name	SBO
GGDP_M	GGDP_M	

Id	Name	SBO

Kinetic Law

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

$$v_5 = \mathrm{kGGTPase} \cdot \mathrm{MgSat10} \cdot [\mathrm{GGTPMg\_M}] \cdot \mathrm{area}\,(\mathrm{M}) \tag{23}$$

Table 20: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
kGGTPase	kGGTPase		1.8	s^{-1}	☑

8.6 Reaction GTPon

This is a reversible reaction of one reactant forming one product influenced by one modifier.

Name GTPon

Reaction equation

$$\mathrm{G\_M} \overset{\mathrm{GTP\_C}}{\rightleftharpoons} \mathrm{GGTP\_M} \tag{24}$$

Reactant

Table 21: Properties of each reactant.

Id	Name	SBO
G_M	G_M	

Modifier

Table 22: Properties of each modifier.

Id	Name	SBO
GTP_C	GTP_C	

Product

Table 23: Properties of each product.

Id	Name	SBO
GGTP_M	GGTP_M	

Kinetic Law

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

$$v_6 = (\text{kGTPon} \cdot [\text{G\_M}] \cdot [\text{GTP\_C}] + ((\text{kGTPoff} \cdot [\text{GGTP\_M}]))) \cdot \text{area}(\text{M}) \tag{25}$$

Table 24: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
kGTPon			0.45	$1 \cdot \mu\text{mol}^{-1} \cdot s^{-1}$	☑
kGTPoff			0.08	s^{-1}	☑

8.7 Reaction GTPgSon

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

Name GTPgSon

Reaction equation

$$9.967 \cdot 10^{-4}\text{GTPgS\_C} + \text{G\_M} \rightleftharpoons \text{GGTPgS\_M} \tag{26}$$

Reactants

Table 25: Properties of each reactant.

Id	Name	SBO
GTPgS_C	GTPgS_C	
G_M	G_M	

Product

Table 26: Properties of each product.

Id	Name	SBO
GGTPgS_M	GGTPgS_M	

Kinetic Law

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

$$v_7 = (\mathrm{kGTPgSon} \cdot [\mathrm{G\_M}] \cdot [\mathrm{GTPgS\_C}] + ((\mathrm{kGTPgSoff} \cdot [\mathrm{GGTPgS\_M}]))) \cdot \mathrm{area}(\mathrm{M}) \quad (27)$$

Table 27: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
kGTPgSon			0.006	$1 \cdot \mu\mathrm{mol}^{-1} \cdot \mathrm{s}^{-1}$	☑
kGTPgSoff			0.005	s^{-1}	☑

8.8 Reaction GDPbSon

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

Name GDPbSon

Reaction equation

$$\mathrm{G\_M} + 9.967 \cdot 10^{-4}\mathrm{GDPbS\_C} \rightleftharpoons \mathrm{GGDPbS\_M} \quad (28)$$

Reactants

Table 28: Properties of each reactant.

Id	Name	SBO
G_M	G_M	
GDPbS_C	GDPbS_C	

Product

Table 29: Properties of each product.

Id	Name	SBO
GGDPbS_M	GGDPbS_M	

Kinetic Law

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

$$v_8 = (\text{kGDPbSon} \cdot [\text{G\_M}] \cdot [\text{GDPbS\_C}] + ((\text{kGGDPbSoff} \cdot (1 + 20 \cdot \text{OxoSat}) \cdot [\text{GGDPbS\_M}]))) \cdot \text{area}(\text{M}) \quad (29)$$

Table 30: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
kGDPbSon			0.28	$1 \cdot \mu\text{mol}^{-1} \cdot \text{s}^{-1}$	☑
kGGDPbSoff			0.10	s^{-1}	☑

8.9 Reaction MgGTPon

This is a reversible reaction of one reactant forming one product influenced by one modifier.

Name MgGTPon

Reaction equation

$$\text{GGTP\_M} \overset{\text{Mg2\_C}}{\rightleftharpoons} \text{GGTPMg\_M} \quad (30)$$

Reactant

Table 31: Properties of each reactant.

Id	Name	SBO
GGTP_M	GGTP_M	

Modifier

Table 32: Properties of each modifier.

Id	Name	SBO
Mg2_C	Mg2_C	

Product

Table 33: Properties of each product.

Id	Name	SBO
GGTPMg_M	GGTPMg_M	

Kinetic Law

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

$$v_9 = \mathrm{kMg2onGTP} \cdot [\mathrm{GGTP\_M}] \cdot [\mathrm{Mg2\_C}] \cdot \mathrm{area}\,(\mathrm{M}) \tag{31}$$

Table 34: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
kMg2onGTP			0.003	$1 \cdot \mu\mathrm{mol}^{-1} \cdot \mathrm{s}^{-1}$	☑

8.10 Reaction GDPdissoc

This is a reversible reaction of one reactant forming two products influenced by one modifier.

Name GDPdissoc

Reaction equation

$$\mathrm{GGDP\_M} \overset{\mathrm{oxoM\_EX}}{\rightleftharpoons} 9.967 \cdot 10^{-4}\mathrm{GDP\_C} + \mathrm{G\_M} \tag{32}$$

Reactant

Table 35: Properties of each reactant.

Id	Name	SBO
GGDP_M	GGDP_M	

Modifier

Table 36: Properties of each modifier.

Id	Name	SBO
oxoM_EX	oxoM_EX	

Products

Table 37: Properties of each product.

Id	Name	SBO
GDP_C	GDP_C	

Id	Name	SBO
G_M	G_M	

Kinetic Law

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

$$v_{10} = (\mathrm{kGDPoff} \cdot [\mathrm{GGDP\_M}] \cdot (\mathrm{OxoSat} + \mathrm{TonicAct}) + ((\mathrm{kGDPon} \cdot [\mathrm{GDP\_C}] \cdot [\mathrm{G\_M}]))) \cdot \mathrm{area}\,(\mathrm{M}) \tag{33}$$

Table 38: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
kGDPoff			0.500	s^{-1}	☑
TonicAct			0.002	dimensionless	☑
kGDPon			0.003	$1 \cdot \mu\mathrm{mol}^{-1} \cdot \mathrm{s}^{-1}$	☑

8.11 Reaction PIP2_5Pase

This is a reversible reaction of one reactant forming one product.

Name PIP2_5Pase

Reaction equation

$$\mathrm{PIP2\_M} \rightleftharpoons \mathrm{PIP\_M} \tag{34}$$

Reactant

Table 39: Properties of each reactant.

Id	Name	SBO
PIP2_M	PIP2_M	

Product

Table 40: Properties of each product.

Id	Name	SBO
PIP_M	PIP_M	

Kinetic Law

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

$$v_{11} = \mathrm{MgSat20} \cdot \mathrm{kPIP2Pase} \cdot [\mathrm{PIP2\_M}] \cdot \mathrm{area}\,(\mathrm{M}) \tag{35}$$

Table 41: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
`kPIP2Pase`			0.005	s^{-1}	☑

8.12 Reaction `PLC`

This is a reversible reaction of one reactant forming one product.

Name PLC

Reaction equation

$$\mathrm{PIP2\_M} \rightleftharpoons 9.967 \cdot 10^{-4} \mathrm{ip3\_C} \tag{36}$$

Reactant

Table 42: Properties of each reactant.

Id	Name	SBO
`PIP2_M`	PIP2_M	

Product

Table 43: Properties of each product.

Id	Name	SBO
`ip3_C`	IP3_C	

Kinetic Law

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

$$v_{12} = \mathrm{kPLC} \cdot (\mathrm{fGactive} + \mathrm{PLCspont}) \cdot [\mathrm{PIP2\_M}] \cdot \mathrm{area}\,(\mathrm{M}) \tag{37}$$

Table 44: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
kPLC			4.800	s^{-1}	☑
PLCspont			$7.5 \cdot 10^{-4}$	dimensionless	☑

8.13 Reaction AlF4on

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

Name AIF4on

Reaction equation

$$9.967 \cdot 10^{-4} \text{AlF4\_C} + \text{GGDP\_M} \rightleftharpoons \text{GGDPAlF4\_M} \tag{38}$$

Reactants

Table 45: Properties of each reactant.

Id	Name	SBO
AlF4_C	AIF4_C	
GGDP_M	GGDP_M	

Product

Table 46: Properties of each product.

Id	Name	SBO
GGDPAlF4_M	GGDPAIF4_M	

Kinetic Law

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

$$v_{13} = (\text{kAlF4on} \cdot [\text{AlF4\_C}] \cdot [\text{GGDP\_M}] + ((\text{kAlF4off} \cdot [\text{GGDPAlF4\_M}]))) \cdot \text{area}(\text{M}) \tag{39}$$

Table 47: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
kAlF4on			$7 \cdot 10^{-6}$	$1 \cdot \mu\text{mol}^{-1} \cdot s^{-1}$	☑
kAlF4off			0.005	s^{-1}	☑

8.14 Reaction PI4Kinase

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

Name PI4Kinase

Reaction equation

$$9.967 \cdot 10^{-4}\,\mathrm{ATP\_C} + \mathrm{PI\_M} \rightleftharpoons \mathrm{PIP\_M} \tag{40}$$

Reactants

Table 48: Properties of each reactant.

Id	Name	SBO
ATP_C	ATP_C	
PI_M	PI_M	

Product

Table 49: Properties of each product.

Id	Name	SBO
PIP_M	PIP_M	

Kinetic Law

Derived unit contains undeclared units

$$v_{14} = (0.2 + 0.8 \cdot \mathrm{MgSat20}) \cdot \mathrm{kPI4Kinase} \cdot [\mathrm{PI\_M}] \cdot \mathrm{ATPSat1000} \cdot \mathrm{area}\,(\mathrm{M}) \tag{41}$$

Table 50: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
kPI4Kinase			10^{-4}	s^{-1}	☑

8.15 Reaction MgonGDPAlF4

This is a reversible reaction of one reactant forming one product influenced by one modifier.

Name MgonGDPAlF4

Reaction equation

$$\text{GGDPAlF4\_M} \overset{\text{Mg2\_C}}{\rightleftharpoons} \text{GGDPAlF4Mg\_M} \tag{42}$$

Reactant

Table 51: Properties of each reactant.

Id	Name	SBO
GGDPAlF4_M	GGDPAIF4_M	

Modifier

Table 52: Properties of each modifier.

Id	Name	SBO
Mg2_C	Mg2_C	

Product

Table 53: Properties of each product.

Id	Name	SBO
GGDPAlF4Mg_M	GGDPAIF4Mg_M	

Kinetic Law

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

$$v_{15} = \mathrm{kMgonAlF4} \cdot [\mathrm{GGDPAlF4\_M}] \cdot [\mathrm{Mg2\_C}] \cdot \mathrm{area}\,(\mathrm{M}) \tag{43}$$

Table 54: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
kMgonAlF4			0.002	$1 \cdot \mu\mathrm{mol}^{-1} \cdot \mathrm{s}^{-1}$	☑

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 GTPgS_C

Name GTPgS_C

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

This species takes part in one reaction (as a reactant in GTPgSon).

$$\frac{\text{d}}{\text{d}t}\text{GTPgS\_C} = -9.967 \cdot 10^{-4} v_7 \tag{44}$$

9.2 Species KCNQsites_M

Name KCNQsites_M

Initial concentration $6.7\ \text{item} \cdot \mu\text{m}^{-2}$

This species takes part in one reaction (as a reactant in PIP2binding).

$$\frac{\text{d}}{\text{d}t}\text{KCNQsites\_M} = -v_3 \tag{45}$$

9.3 Species PIP2_M

Name PIP2_M

Initial concentration $5000\ \text{item} \cdot \mu\text{m}^{-2}$

This species takes part in four reactions (as a reactant in PIP2binding, PIP2_5Pase, PLC and as a product in PIP5kinase).

$$\frac{\text{d}}{\text{d}t}\text{PIP2\_M} = v_1 - v_3 - v_{11} - v_{12} \tag{46}$$

9.4 Species GGDPbS_M

Name GGDPbS_M

Initial concentration $0\ \text{item} \cdot \mu\text{m}^{-2}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{GGDPbS\_M} = v_8 \tag{47}$$

9.5 Species Mg2_C

Name Mg2_C

Initial concentration $2100\ \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in three reactions (as a modifier in MgonGGTPgS, MgGTPon, MgonGDPAlF4), which do not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{Mg2\_C} = 0 \tag{48}$$

9.6 Species ATP_C

Name ATP_C

Initial concentration $3000\ \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a reactant in PIP5kinase, PI4Kinase).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{ATP\_C} = -9.967 \cdot 10^{-4}\, v_1 - 9.967 \cdot 10^{-4} v_{14} \tag{49}$$

9.7 Species oxoM_EX

Name oxoM_EX

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

Involved in events event_0000001, event_0000002

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{oxoM\_EX} = 0 \tag{50}$$

Furthermore, two events influence this species' rate of change.

9.8 Species GDPbS_C

Name GDPbS_C

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

This species takes part in one reaction (as a reactant in GDPbSon).

$$\frac{\text{d}}{\text{d}t}\text{GDPbS\_C} = -9.967 \cdot 10^{-4} v_8 \tag{51}$$

9.9 Species GGTPMg_M

Name GGTPMg_M

Initial concentration $0.1\ \text{item} \cdot \mu\text{m}^{-2}$

This species takes part in two reactions (as a reactant in GGTPase and as a product in MgGTPon).

$$\frac{\text{d}}{\text{d}t}\text{GGTPMg\_M} = v_9 - v_5 \tag{52}$$

9.10 Species GDP_C

Name GDP_C

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

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

$$\frac{\text{d}}{\text{d}t}\text{GDP\_C} = 9.967 \cdot 10^{-4} v_{10} \tag{53}$$

9.11 Species GTP_C

Name GTP_C

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

Involved in rule GTP_C

This species takes part in one reaction (as a modifier in GTPon) and is also involved in one rule which determines this species' quantity.

9.12 Species GGDPAlF4Mg_M

Name GGDPAIF4Mg_M

Initial concentration $0\ \text{item} \cdot \mu\text{m}^{-2}$

This species takes part in one reaction (as a product in MgonGDPAlF4).

$$\frac{\text{d}}{\text{d}t}\text{GGDPAlF4Mg\_M} = v_{15} \tag{54}$$

9.13 Species ip3_C

Name IP3_C

Initial concentration $0.48\ \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a reactant in IP3Phosphatase and as a product in PLC).

$$\frac{\text{d}}{\text{d}t}\text{ip3\_C} = 9.967 \cdot 10^{-4} v_{12} - 1.666111296 \cdot 10^{-18} v_2 \tag{55}$$

9.14 Species AlF4_C

Name AIF4_C

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

This species takes part in one reaction (as a reactant in AlF4on).

$$\frac{\text{d}}{\text{d}t}\text{AlF4\_C} = -9.967 \cdot 10^{-4} v_{13} \tag{56}$$

9.15 Species G_M

Name G_M

Initial concentration $0.065\ \text{item} \cdot \mu\text{m}^{-2}$

This species takes part in four reactions (as a reactant in GTPon, GTPgSon, GDPbSon and as a product in GDPdissoc).

$$\frac{\text{d}}{\text{d}t}\text{G\_M} = v_{10} - v_6 - v_7 - v_8 \tag{57}$$

9.16 Species GGTP_M

Name GGTP_M

Initial concentration $0.048\ \text{item} \cdot \mu\text{m}^{-2}$

This species takes part in two reactions (as a reactant in MgGTPon and as a product in GTPon).

$$\frac{\text{d}}{\text{d}t}\text{GGTP\_M} = v_6 - v_9 \tag{58}$$

9.17 Species GGDPAlF4_M

Name GGDPAIF4_M

Initial concentration $0\ \text{item} \cdot \mu\text{m}^{-2}$

This species takes part in two reactions (as a reactant in MgonGDPAlF4 and as a product in AlF4on).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{GGDPAlF4\_M} = v_{13} - v_{15} \tag{59}$$

9.18 Species GGTPgS_M

Name GGTPgS_M

Initial concentration $0\ \text{item} \cdot \mu\text{m}^{-2}$

This species takes part in two reactions (as a reactant in MgonGGTPgS and as a product in GTPgSon).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{GGTPgS\_M} = v_7 - v_4 \tag{60}$$

9.19 Species PI_M

Name PI_M

Initial concentration $200000\ \text{item} \cdot \mu\text{m}^{-2}$

This species takes part in one reaction (as a reactant in PI4Kinase).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{PI\_M} = -v_{14} \tag{61}$$

9.20 Species PIP_M

Name PIP_M

Initial concentration $1150\ \text{item} \cdot \mu\text{m}^{-2}$

This species takes part in three reactions (as a reactant in PIP5kinase and as a product in PIP2_5Pase, PI4Kinase).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{PIP\_M} = v_{11} + v_{14} - v_1 \tag{62}$$

9.21 Species PIP2xKCNQ_M

Name PIP2xKCNQ_M

Initial concentration $33.3\ \text{item} \cdot \mu\text{m}^{-2}$

This species takes part in one reaction (as a product in PIP2binding).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{PIP2xKCNQ\_M} = v_3 \tag{63}$$

9.22 Species GGTPgSMg_M

Name GGTPgSMg_M

Initial concentration $0\ \text{item} \cdot \mu\text{m}^{-2}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{GGTPgSMg\_M} = v_4 \tag{64}$$

9.23 Species GGDP_M

Name GGDP_M

Initial concentration $200\ \text{item} \cdot \mu\text{m}^{-2}$

This species takes part in three reactions (as a reactant in GDPdissoc, AlF4on and as a product in GGTPase).

$$\frac{\mathrm{d}}{\mathrm{d}t}\text{GGDP\_M} = v_5 - v_{10} - v_{13} \tag{65}$$

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