

## SBML Model Report

**Model name:**  
**“Chan2004\_TCell\_receptor\_activation”**



May 6, 2016

### 1 General Overview

This is a document in SBML Level 2 Version 1 format. This model was created by Harish Dharuri<sup>1</sup> at June 22<sup>nd</sup> 2007 at 1:48 a. m. and last time modified at April eighth 2016 at 3:36 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	1
species types	0	species	5
events	2	constraints	0
reactions	10	function definitions	0
global parameters	11	unit definitions	4
rules	1	initial assignments	0

### Model Notes

The model reproduces Fig 3a of the paper. Please note that the authors mention that they used a value of 2 for  $n$ ,  $n$  being the power in the positive feedback function for kinase autocatalysis, however the model here has  $n=1.95$  because this results in a simulation that is identical to Fig 3a. The model was successfully tested on MathSBML.

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## 2 Unit Definitions

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

### 2.1 Unit `substance`

**Definition** `item`

### 2.2 Unit `items_per_time`

**Name** `items_per_time`

**Definition**  $\text{item} \cdot \text{s}^{-1}$

### 2.3 Unit `sec_inv`

**Name** `sec_inv`

**Definition**  $\text{s}^{-1}$

### 2.4 Unit `sec_inv_item_inv`

**Name** `per_sec_per_item`

**Definition**  $\text{item}^{-1} \cdot \text{s}^{-1}$

### 2.5 Unit `volume`

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

**Definition** `l`

## 2.6 Unit area

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

**Definition**  $\text{m}^2$

## 2.7 Unit length

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

**Definition** m

## 2.8 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
compartment	cell		3	1	litre	<input checked="" type="checkbox"/>	

## 3.1 Compartment `compartment`

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

**Name** cell

## 4 Species

This model contains five species. 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
lck_inactive	Inactive lck	compartment	item	$\square$	$\square$
lck_active	Active lck	compartment	item	$\square$	$\square$
phosphatase- _inactive	Inactive phosphatase	compartment	item	$\square$	$\square$
phosphatase- _active	Active phosphatase	compartment	item	$\square$	$\square$
lck_total	Total kinase	compartment	item	$\square$	$\square$

## 5 Parameters

This model contains eleven global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
n1			1.00	item <sup>-1</sup> · s <sup>-1</sup>	<input checked="" type="checkbox"/>
k1			0.01	s <sup>-1</sup>	<input checked="" type="checkbox"/>
m1			1.00		<input checked="" type="checkbox"/>
d0			0.15	s <sup>-1</sup>	<input checked="" type="checkbox"/>
d1			0.15	s <sup>-1</sup>	<input checked="" type="checkbox"/>
k2			0.01	s <sup>-1</sup>	<input checked="" type="checkbox"/>
m2			1.00	item <sup>-1</sup> · s <sup>-1</sup>	<input checked="" type="checkbox"/>
n2			0.02	s <sup>-1</sup>	<input checked="" type="checkbox"/>
d2			0.00	s <sup>-1</sup>	<input checked="" type="checkbox"/>
n			1.95	dimensionless	<input checked="" type="checkbox"/>
r_1			0.00	item · s <sup>-1</sup>	<input type="checkbox"/>

## 6 Rule

This is an overview of one rule.

### 6.1 Rule lck\_total

Rule lck\_total is an assignment rule for species lck\_total:

$$[\text{lck\_total}] = \text{lck\_inactive} + \text{lck\_active} \quad (1)$$

**Derived unit** item

## 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

**Name** Setting r(l) to 1

**Trigger condition**

$$t \geq 10 \quad (2)$$

**Assignment**

$$r.l = 1 \quad (3)$$

## 7.2 Event `event_0000002`

**Name** Resetting  $r(l)$  to 0

**Trigger condition**

$$t \geq 24 \quad (4)$$

**Assignment**

$$r.l = 0 \quad (5)$$

## 8 Reactions

This model contains ten 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

Nº	Id	Name	Reaction Equation	SBO
1	v1	Kinase recruitment to T-cell receptor	$\emptyset \longrightarrow \text{lck\_inactive}$	
2	v2	Kinase inactivation	$\text{lck\_active} \xrightarrow{\text{phosphatase\_active}} \text{lck\_inactive}$	
3	v3	Basal kinase activation	$\text{lck\_inactive} \longrightarrow \text{lck\_active}$	
4	v4	Catalytic kinase activation	$\text{lck\_inactive} \longrightarrow \text{lck\_active}$	
5	v5	Inactive kinase diffusion	$\text{lck\_inactive} \longrightarrow \emptyset$	
6	v6	Active kinase diffusion	$\text{lck\_active} \longrightarrow \emptyset$	
7	v7	Basal phosphatase activation	$\text{phosphatase\_inactive} \longrightarrow \text{phosphatase\_active}$	
8	v8	Catalyzed phosphatase activation	$\text{phosphatase\_inactive} \xrightarrow{\text{lck\_active}} \text{phosphatase\_active}$	
9	v9	Phosphatase inactivation	$\text{phosphatase\_active} \longrightarrow \text{phosphatase\_inactive}$	
10	v10	Active phosphatase diffusion	$\text{phosphatase\_active} \longrightarrow \emptyset$	

### 8.1 Reaction $v_1$

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

**Name** Kinase recruitment to T-cell receptor

#### Reaction equation



#### Product

Table 6: Properties of each product.

Id	Name	SBO
<code>lck_inactive</code>	Inactive lck	

#### Kinetic Law

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

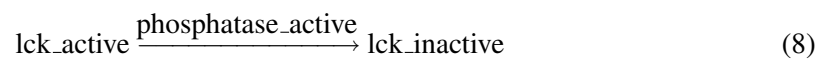
$$v_1 = r_1 \quad (7)$$

### 8.2 Reaction $v_2$

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

**Name** Kinase inactivation

#### Reaction equation



#### Reactant

Table 7: Properties of each reactant.

Id	Name	SBO
<code>lck_active</code>	Active lck	

#### Modifier



Table 8: Properties of each modifier.

Id	Name	SBO
phosphatase_active	Active phosphatase	

## Product

Table 9: Properties of each product.

Id	Name	SBO
lck_inactive	Inactive lck	

## Kinetic Law

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

$$v_2 = n_1 \cdot \text{lck\_active} \cdot \text{phosphatase\_active} \quad (9)$$

## 8.3 Reaction v3

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

**Name** Basal kinase activation

## Reaction equation



## Reactant

Table 10: Properties of each reactant.

Id	Name	SBO
lck_inactive	Inactive lck	

## Product

Table 11: Properties of each product.

Id	Name	SBO
lck_active	Active lck	

### Kinetic Law

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

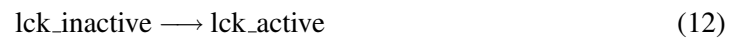
$$v_3 = k1 \cdot \text{lck\_inactive} \quad (11)$$

### 8.4 Reaction $v_4$

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

**Name** Catalytic kinase activation

### Reaction equation



### Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
<code>lck_inactive</code>	Inactive lck	

### Product

Table 13: Properties of each product.

Id	Name	SBO
<code>lck_active</code>	Active lck	

### Kinetic Law

**Derived unit** contains undeclared units

$$v_4 = m1 \cdot \text{lck\_active}^n \cdot \text{lck\_inactive} \quad (13)$$

### 8.5 Reaction $v_5$

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

**Name** Inactive kinase diffusion

### Reaction equation



## Reactant

Table 14: Properties of each reactant.

Id	Name	SBO
<code>lck_inactive</code>	Inactive lck	

## Kinetic Law

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

$$v_5 = d0 \cdot \text{lck\_inactive} \quad (15)$$

## 8.6 Reaction $v_6$

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

**Name** Active kinase diffusion

## Reaction equation



## Reactant

Table 15: Properties of each reactant.

Id	Name	SBO
<code>lck_active</code>	Active lck	

## Kinetic Law

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

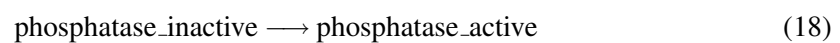
$$v_6 = d1 \cdot \text{lck\_active} \quad (17)$$

## 8.7 Reaction $v_7$

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

**Name** Basal phosphatase activation

## Reaction equation



## Reactant

Table 16: Properties of each reactant.

Id	Name	SBO
phosphatase_inactive	Inactive phosphatase	

## Product

Table 17: Properties of each product.

Id	Name	SBO
phosphatase_active	Active phosphatase	

## Kinetic Law

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

$$v_7 = k_2 \cdot \text{phosphatase\_inactive} \quad (19)$$

## 8.8 Reaction v8

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

**Name** Catalyzed phosphatase activation

## Reaction equation



## Reactant

Table 18: Properties of each reactant.

Id	Name	SBO
phosphatase_inactive	Inactive phosphatase	

## Modifier

Table 19: Properties of each modifier.

Id	Name	SBO
<code>lck_active</code>	Active lck	

## Product

Table 20: Properties of each product.

Id	Name	SBO
<code>phosphatase_active</code>	Active phosphatase	

## Kinetic Law

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

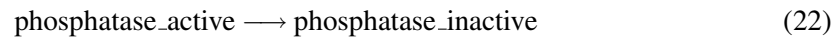
$$v_8 = m_2 \cdot \text{lck\_active} \cdot \text{phosphatase\_inactive} \quad (21)$$

## 8.9 Reaction $v_9$

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

**Name** Phosphatase inactivation

## Reaction equation



## Reactant

Table 21: Properties of each reactant.

Id	Name	SBO
<code>phosphatase_active</code>	Active phosphatase	

## Product

Table 22: Properties of each product.

Id	Name	SBO
<code>phosphatase_inactive</code>	Inactive phosphatase	

### Kinetic Law

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

$$v_9 = n2 \cdot \text{phosphatase\_active} \quad (23)$$

### 8.10 Reaction $v_{10}$

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

**Name** Active phosphatase diffusion

### Reaction equation



### Reactant

Table 23: Properties of each reactant.

Id	Name	SBO
phosphatase_active	Active phosphatase	

### Kinetic Law

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

$$v_{10} = d2 \cdot \text{phosphatase\_active} \quad (25)$$

## 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 `lck_inactive`

**Name** Inactive lck

**Initial amount** 0 item

This species takes part in five reactions (as a reactant in `v3`, `v4`, `v5` and as a product in `v1`, `v2`).

$$\frac{d}{dt}lck\_inactive = v_1 + v_2 - v_3 - v_4 - v_5 \quad (26)$$

### 9.2 Species `lck_active`

**Name** Active lck

**Initial amount** 0 item

This species takes part in five reactions (as a reactant in `v2`, `v6` and as a product in `v3`, `v4` and as a modifier in `v8`).

$$\frac{d}{dt}lck\_active = v_3 + v_4 - v_2 - v_6 \quad (27)$$

### 9.3 Species `phosphatase_inactive`

**Name** Inactive phosphatase

**Initial amount** 0.6 item

This species takes part in three reactions (as a reactant in `v7`, `v8` and as a product in `v9`).

$$\frac{d}{dt}phosphatase\_inactive = v_9 - v_7 - v_8 \quad (28)$$

### 9.4 Species `phosphatase_active`

**Name** Active phosphatase

**Initial amount** 0.6 item

This species takes part in five reactions (as a reactant in `v9`, `v10` and as a product in `v7`, `v8` and as a modifier in `v2`).

$$\frac{d}{dt}phosphatase\_active = v_7 + v_8 - v_9 - v_{10} \quad (29)$$

### 9.5 Species `lck_total`

**Name** Total kinase

**Initial amount** 0 item

**Involved in rule** `lck_total`

One rule which determines this species' quantity.

SBML<sup>2</sup>TeX was developed by Andreas Dräger<sup>a</sup>, Hannes Planatscher<sup>a</sup>, Dieudonné M Wouamba<sup>a</sup>, Adrian Schröder<sup>a</sup>, Michael Hucka<sup>b</sup>, Lukas Endler<sup>c</sup>, Martin Golebiewski<sup>d</sup> and Andreas Zell<sup>a</sup>. Please see <http://www.ra.cs.uni-tuebingen.de/software/SBML2LaTeX> for more information.

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