SBML Model Report

Model name: "Markevich2004_MAPK_orderedElementary"

May 5, 2016

1 General Overview

This is a document in SBML Level 2 Version 1 format. This model was created by the following two authors: Nicolas Le Novre[1] and Rainer Machne[2] at May 23rd 2005 at 12:47 a. m. and last time modified at May 15th 2012 at 9:41 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	11
events	0	constraints	0
reactions	10	function definitions	0
global parameters	16	unit definitions	1
rules	0	initial assignments	0

Model Notes

The model corresponds to the schemas 1 and 2 of Markevich et al 2004, as described in the figure 1 and the supplementary table S1. Phosphorylations and dephosphorylations follow distributive ordered kinetics. The phosphorylations are modeled with three elementary reactions:
E+S<=>ES->E+P

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The dephosphorylations are modeled with five elementary reactions:
E+S<=>ES->EP<=>E+P

2 Unit Definitions

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

2.1 Unit `substance`

Name nanomole (default)

Definition nmol

2.2 Unit `volume`

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

Definition l

2.3 Unit `area`

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

Definition m^2

2.4 Unit `length`

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

Definition m

2.5 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
uVol			3	1	litre	☑	

3.1 Compartment uVol

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

4 Species

This model contains eleven 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 Condition
M		uVol	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Mp		uVol	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Mpp		uVol	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
MAPKK		uVol	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
MKP3	MKP	uVol	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
M_MAPKK		uVol	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Mp_MAPKK		uVol	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Mpp_MKP3	Mpp_MKP	uVol	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Mp_MKP3_dep	Mp_MKP	uVol	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
Mp_MKP3	Mp_MKP*	uVol	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟
M_MKP3	M_MKP	uVol	$\mathrm{nmol} \cdot \mathrm{l}^{-1}$	⊟	⊟

5 Parameters

This model contains 16 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k1			0.020		☑
k_1			1.000		☑
k2			0.010		☑
k3			0.032		☑
k_3			1.000		☑
k4			15.000		☑
h1			0.045		☑
h_1			1.000		☑
h2			0.092		☑
h3			1.000		☑
h_3			0.010		☑
h4			0.010		☑
h_4			1.000		☑
h5			0.500		☑
h6			0.086		☑
h_6			0.001		☑

6 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

№	Id	Name	Reaction Equation	SBO
1	v1a	binding MAPK and PP-MAPKK	$M + MAPKK \rightleftharpoons M\_MAPKK$	
2	v1b	phosphorylation of MAPK	$M\_MAPKK \longrightarrow Mp + MAPKK$	
3	v2a	binding PP-MAPKK and P-MAPK	$Mp + MAPKK \rightleftharpoons Mp\_MAPKK$	
4	v2b	phosphorylation of P-MAPK	$Mp\_MAPKK \longrightarrow Mpp + MAPKK$	
5	v3a	binding MKP and PP-MAPK	$Mpp + MKP3 \rightleftharpoons Mpp\_MKP3$	
6	v3b	dephosphorylation of PP-MAPK	$Mpp\_MKP3 \longrightarrow Mp\_MKP3\_dep$	
7	v3c	dissociation of MKP from P-MAPK	$Mp\_MKP3\_dep \rightleftharpoons Mp + MKP3$	
8	v4a	binding MKP and P-MAPK	$Mp + MKP3 \rightleftharpoons Mp\_MKP3$	
9	v4b	dephosphorylation of P-MAPK	$Mp\_MKP3 \longrightarrow M\_MKP3$	
10	v4c	dissociation of MKP from MAPK	$M\_MKP3 \rightleftharpoons M + MKP3$	

6.1 Reaction v1a

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

Name binding MAPK and PP-MAPKK

Reaction equation

$$\mathrm{M} + \mathrm{MAPKK} \rightleftharpoons \mathrm{M\_MAPKK} \tag{1}$$

Reactants

Table 6: Properties of each reactant.

Id	Name	SBO
M		
MAPKK		

Product

Table 7: Properties of each product.

Id	Name	SBO
M_MAPKK		

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \mathrm{vol}\,(\mathrm{uVol}) \cdot (\mathrm{k1} \cdot [\mathrm{M}] \cdot [\mathrm{MAPKK}] - \mathrm{k\_1} \cdot [\mathrm{M\_MAPKK}]) \tag{2}$$

6.2 Reaction v1b

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

Name phosphorylation of MAPK

Reaction equation

$$\mathrm{M\_MAPKK} \longrightarrow \mathrm{Mp} + \mathrm{MAPKK} \tag{3}$$

Reactant

Table 8: Properties of each reactant.

Id	Name	SBO
M_MAPKK		

Products

Table 9: Properties of each product.

Id	Name	SBO
Mp		
MAPKK		

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \mathrm{vol}\,(\mathrm{uVol}) \cdot \mathrm{k2} \cdot [\mathrm{M\_MAPKK}] \tag{4}$$

6.3 Reaction v2a

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

Name binding PP-MAPKK and P-MAPK

Reaction equation

$$\mathrm{Mp} + \mathrm{MAPKK} \rightleftharpoons \mathrm{Mp\_MAPKK} \tag{5}$$

Reactants

Table 10: Properties of each reactant.

Id	Name	SBO
Mp		
MAPKK		

Product

Table 11: Properties of each product.

Id	Name	SBO
Mp_MAPKK		

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \mathrm{vol}\,(\mathrm{uVol}) \cdot (\mathrm{k3} \cdot [\mathrm{Mp}] \cdot [\mathrm{MAPKK}] - \mathrm{k\_3} \cdot [\mathrm{Mp\_MAPKK}]) \tag{6}$$

6.4 Reaction v2b

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

Name phosphorylation of P-MAPK

Reaction equation

$$\mathrm{Mp\_MAPKK} \longrightarrow \mathrm{Mpp} + \mathrm{MAPKK} \tag{7}$$

Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
Mp_MAPKK		

Products

Table 13: Properties of each product.

Id	Name	SBO
Mpp		
MAPKK		

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \mathrm{vol}\,(\mathrm{uVol}) \cdot \mathrm{k4} \cdot [\mathrm{Mp\_MAPKK}] \tag{8}$$

6.5 Reaction v3a

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

Name binding MKP and PP-MAPK

Reaction equation

$$\mathrm{Mpp} + \mathrm{MKP3} \rightleftharpoons \mathrm{Mpp\_MKP3} \tag{9}$$

Reactants

Table 14: Properties of each reactant.

Id	Name	SBO
Mpp		
MKP3	MKP	

Product

Table 15: Properties of each product.

Id	Name	SBO
Mpp_MKP3	Mpp_MKP	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \mathrm{vol}\,(\mathrm{uVol}) \cdot (\mathrm{h1} \cdot [\mathrm{Mpp}] \cdot [\mathrm{MKP3}] - \mathrm{h\_1} \cdot [\mathrm{Mpp\_MKP3}]) \tag{10}$$

6.6 Reaction v3b

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

Name dephosphorylation of PP-MAPK

Reaction equation

$$\mathrm{Mpp\_MKP3} \longrightarrow \mathrm{Mp\_MKP3\_dep} \tag{11}$$

Reactant

Table 16: Properties of each reactant.

Id	Name	SBO
Mpp_MKP3	Mpp_MKP	

Product

Table 17: Properties of each product.

Id	Name	SBO
Mp_MKP3_dep	Mp_MKP	

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \mathrm{vol}\,(\mathrm{uVol}) \cdot \mathrm{h2} \cdot [\mathrm{Mpp\_MKP3}] \tag{12}$$

6.7 Reaction v3c

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

Name dissociation of MKP from P-MAPK

Reaction equation

$$\mathrm{Mp\_MKP3\_dep} \rightleftharpoons \mathrm{Mp} + \mathrm{MKP3} \tag{13}$$

Reactant

Table 18: Properties of each reactant.

Id	Name	SBO
Mp_MKP3_dep	Mp_MKP	

Products

Table 19: Properties of each product.

Id	Name	SBO
Mp		
MKP3	MKP	

Id	Name	SBO

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \mathrm{h3} \cdot [\mathrm{Mp\_MKP3\_dep}] - \mathrm{h\_3} \cdot [\mathrm{Mp}] \cdot [\mathrm{MKP3}] \tag{14}$$

6.8 Reaction v4a

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

Name binding MKP and P-MAPK

Reaction equation

$$\mathrm{Mp} + \mathrm{MKP3} \rightleftharpoons \mathrm{Mp\_MKP3} \tag{15}$$

Reactants

Table 20: Properties of each reactant.

Id	Name	SBO
Mp		
MKP3	MKP	

Product

Table 21: Properties of each product.

Id	Name	SBO
Mp_MKP3	Mp_MKP*	

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \mathrm{vol}\,(\mathrm{uVol}) \cdot (\mathrm{h4} \cdot [\mathrm{Mp}] \cdot [\mathrm{MKP3}] - \mathrm{h\_4} \cdot [\mathrm{Mp\_MKP3}]) \tag{16}$$

6.9 Reaction v4b

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

Name dephosphorylation of P-MAPK

Reaction equation

$$\text{Mp\_MKP3} \longrightarrow \text{M\_MKP3} \tag{17}$$

Reactant

Table 22: Properties of each reactant.

Id	Name	SBO
Mp_MKP3	Mp_MKP*	

Product

Table 23: Properties of each product.

Id	Name	SBO
M_MKP3	M_MKP	

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \text{vol}\left(\text{uVol}\right) \cdot \text{h5} \cdot \left[\text{Mp\_MKP3}\right] \tag{18}$$

6.10 Reaction v4c

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

Name dissociation of MKP from MAPK

Reaction equation

$$\text{M\_MKP3} \rightleftharpoons \text{M} + \text{MKP3} \tag{19}$$

Reactant

Table 24: Properties of each reactant.

Id	Name	SBO
M_MKP3	M_MKP	

Products

Table 25: Properties of each product.

Id	Name	SBO
M		
MKP3	MKP	

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = \mathrm{vol}\,(\mathrm{uVol}) \cdot (\mathrm{h6} \cdot [\mathrm{M\_MKP3}] - \mathrm{h\_6} \cdot [\mathrm{M}] \cdot [\mathrm{MKP3}]) \tag{20}$$

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.

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.

7.1 Species `M`

Initial amount 500 nmol

This species takes part in two reactions (as a reactant in `v1a` and as a product in `v4c`).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{M} = v_{10} - v_1 \tag{21}$$

7.2 Species `Mp`

Initial amount 0 nmol

This species takes part in four reactions (as a reactant in `v2a`, `v4a` and as a product in `v1b`, `v3c`).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Mp} = v_2 + v_7 - v_3 - v_8 \tag{22}$$

7.3 Species Mpp

Initial amount 0 nmol

This species takes part in two reactions (as a reactant in v3a and as a product in v2b).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Mpp} = v_4 - v_5 \tag{23}$$

7.4 Species MAPKK

Initial amount 50 nmol

This species takes part in four reactions (as a reactant in v1a, v2a and as a product in v1b, v2b).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{MAPKK} = v_2 + v_4 - v_1 - v_3 \tag{24}$$

7.5 Species MKP3

Name MKP

Initial amount 100 nmol

This species takes part in four reactions (as a reactant in v3a, v4a and as a product in v3c, v4c).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{MKP3} = v_7 + v_{10} - v_5 - v_8 \tag{25}$$

7.6 Species M_MAPKK

Initial amount 0 nmol

This species takes part in two reactions (as a reactant in v1b and as a product in v1a).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{M\_MAPKK} = v_1 - v_2 \tag{26}$$

7.7 Species Mp_MAPKK

Initial amount 0 nmol

This species takes part in two reactions (as a reactant in v2b and as a product in v2a).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Mp\_MAPKK} = v_3 - v_4 \tag{27}$$

7.8 Species Mpp_MKP3

Name Mpp_MKP

Initial amount 0 nmol

This species takes part in two reactions (as a reactant in v3b and as a product in v3a).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Mpp\_MKP3} = v_5 - v_6 \tag{28}$$

7.9 Species Mp_MKP3_dep

Name Mp_MKP

Initial amount 0 nmol

This species takes part in two reactions (as a reactant in v3c and as a product in v3b).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Mp\_MKP3\_dep} = v_6 - v_7 \tag{29}$$

7.10 Species Mp_MKP3

Name Mp_MKP*

Initial amount 0 nmol

This species takes part in two reactions (as a reactant in v4b and as a product in v4a).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Mp\_MKP3} = v_8 - v_9 \tag{30}$$

7.11 Species M_MKP3

Name M_MKP

Initial amount 0 nmol

This species takes part in two reactions (as a reactant in v4c and as a product in v4b).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{M\_MKP3} = v_9 - v_{10} \tag{31}$$

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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