SBML Model Report

Model name: "Kolomeisky2003_MyosinV_Processivity"

May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by Lukas Endler[1] at September 29th 2006 at 10:36 p. m. and last time modified at April eighth 2016 at 4:58 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	9
events	0	constraints	0
reactions	4	function definitions	0
global parameters	15	unit definitions	4
rules	4	initial assignments	0

Model Notes

This is the 2 state model of Myosin V movement described in the article:
A simple kinetic model describes the processivity of myosin-v.
Kolomeisky AB , Fisher ME Biophys. J. 84(3):1642-50 (2003); PubmedID:12609867

Abstract:
Myosin-V is a motor protein responsible for organelle and vesicle transport in cells. Recent

[1]EMBL-EBI, lukas@ebi.ac.uk

single-molecule experiments have shown that it is an efficient processive motor that walks along actin filaments taking steps of mean size close to 36 nm. A theoretical study of myosin-V motility is presented following an approach used successfully to analyze the dynamics of conventional kinesin but also taking some account of step-size variations. Much of the present experimental data for myosin-V can be well described by a two-state chemical kinetic model with three load-dependent rates. In addition, the analysis predicts the variation of the mean velocity and of the randomness-a quantitative measure of the stochastic deviations from uniform, constant-speed motion-with ATP concentration under both resisting and assisting loads, and indicates a substep of size d(0) approximately 13-14 nm (from the ATP-binding state) that appears to accord with independent observations.

The model differs slightly from the published version. The ATP and ADP bound forms of myosin are called S0 and S1. The state transition and binding constants are called k_1, k_2, k_3 and k_4 instead of $k^0{}_0$, $u^0{}_1$, k'_0 and $w^0{}_1$. Similarly the state loading factors are named th_1, th_2, th_3 and th_4 instead of $^+{}_0$, $^+{}_1$, $^-{}_0$ and $^-{}_1$. The species fwd_step1, fwd_step2, back_step1 and back_step2 count the number of state changes of each kind the myosine molecules have taken over time.

The model can be evaluated in a deterministic continuous or stochastic discreet fashion. The parameter V holds the (forward) speed at each time point, the V_avg the overall way divided by the simulation time and the amount of myosine molecules.

Originally created by libAntimony v1.4 (using libSBML 3.4.1)

2 Unit Definitions

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

2.1 Unit `substance`

Name molecules

Definition item

2.2 Unit `umole`

Name micromole

Definition μmol

2.3 Unit uM

Name uM

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

2.4 Unit volume

Name litre

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
compartment_		0000290	3	10^{-15}	l	☑	

3.1 Compartment compartment_

This is a three dimensional compartment with a constant size of 10^{-15} litre.

SBO:0000290 physical compartment

4 Species

This model contains nine species. The boundary condition of three of these species is set to `true` so that these species' amount cannot be changed by any reaction. 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
S0		compartment_	item	☐	☐
ATP		compartment_	$\mu mol \cdot l^{-1}$	☐	☑
S1		compartment_	item	☐	☐
Pi_		compartment_	$\mu mol \cdot l^{-1}$	☐	☑
ADP		compartment_	$\mu mol \cdot l^{-1}$	☐	☑
fwd_step1		compartment_	item	☐	☐
fwd_step2		compartment_	item	☐	☐
back_step1		compartment_	item	☐	☐
back_step2		compartment_	item	☐	☐

5 Parameters

This model contains 15 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
k_1		0000023	0.700		☑
th_1		0000380	−0.010		☑
Force			0.000		☑
d		0000466	36.000		☑
kT			4.116		☑
k_2		0000022	12.000		☑
th_2		0000380	0.045		☑
k_3		0000023	$5 \cdot 10^{-6}$		☑
th_3		0000380	0.580		☑
k_4		0000022	$6 \cdot 10^{-6}$		☑
th_4		0000380	0.385		☑
S_tot		0000360	0.000		⊟
V			0.000		⊟
V_ave			0.000		⊟
tau		0000347	0.000		⊟

6 Rules

This is an overview of four rules.

6.1 Rule S_tot

Rule S_tot is an assignment rule for parameter S_tot:

$$\mathrm{S\_tot} = \mathrm{S0} + \mathrm{S1} \tag{1}$$

Derived unit item

6.2 Rule V

Rule V is an assignment rule for parameter V:

$$\mathrm{V} = \frac{\mathrm{d} \cdot \left(\frac{\mathrm{Fw\_1st\_step} + \mathrm{Fw\_2nd\_step}}{2} - \frac{\mathrm{Bw\_1st\_step} + \mathrm{Bw\_2nd\_step}}{2} \right)}{\mathrm{S\_tot}} \tag{2}$$

6.3 Rule V_ave

Rule V_ave is an assignment rule for parameter V_ave:

$$\mathrm{V\_ave} = \frac{\mathrm{d} \cdot \left(\frac{\mathrm{fwd\_step1} + \mathrm{fwd\_step2}}{2} - \frac{\mathrm{back\_step1} + \mathrm{back\_step2}}{2} \right)}{\mathrm{S\_tot} \cdot \mathrm{time}} \tag{3}$$

6.4 Rule tau

Rule tau is an assignment rule for parameter tau:

$$\mathrm{tau} = \frac{\mathrm{k\_1} \cdot [\mathrm{ATP}] \cdot \exp\left(\frac{\mathrm{th\_1} \cdot \mathrm{Force} \cdot \mathrm{d}}{\mathrm{kT}}\right) + \mathrm{k\_2} \cdot \exp\left(\frac{\mathrm{th\_2} \cdot \mathrm{Force} \cdot \mathrm{d}}{\mathrm{kT}}\right) + \mathrm{k\_3} \cdot [\mathrm{ATP}] \cdot \exp\left(\frac{\mathrm{th\_3} \cdot \mathrm{Force} \cdot \mathrm{d}}{\mathrm{kT}}\right) + \mathrm{k\_4} \cdot \exp\left(\frac{\mathrm{th\_4} \cdot \mathrm{Force} \cdot \mathrm{d}}{\mathrm{kT}}\right)}{\mathrm{k\_1} \cdot [\mathrm{ATP}] \cdot \exp\left(\frac{\mathrm{th\_1} \cdot \mathrm{Force} \cdot \mathrm{d}}{\mathrm{kT}}\right) \cdot \mathrm{k\_2} \cdot \exp\left(\frac{\mathrm{th\_2} \cdot \mathrm{Force} \cdot \mathrm{d}}{\mathrm{kT}}\right) + \mathrm{k\_3} \cdot [\mathrm{ATP}] \cdot \exp\left(\frac{\mathrm{th\_3} \cdot \mathrm{Force} \cdot \mathrm{d}}{\mathrm{kT}}\right) \cdot \mathrm{k\_4} \cdot \exp\left(\frac{\mathrm{th\_4} \cdot \mathrm{Force} \cdot \mathrm{d}}{\mathrm{kT}}\right)} \tag{4}$$

7 Reactions

This model contains four 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	`Fw_1st_step`		$S0 + ATP \longrightarrow S1 + Pi\_ + fwd\_step1$	0000376
2	`Fw_2nd_step`		$S1 \longrightarrow S0 + ADP + fwd\_step2$	0000180
3	`Bw_1st_step`		$S0 + ATP \longrightarrow S1 + Pi\_ + back\_step1$	0000376
4	`Bw_2nd_step`		$S1 \longrightarrow S0 + ADP + back\_step2$	0000180

7.1 Reaction Fw_1st_step

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

SBO:0000376 hydrolysis

Reaction equation

$$\mathrm{S0} + \mathrm{ATP} \longrightarrow \mathrm{S1} + \mathrm{Pi\_} + \mathrm{fwd\_step1} \tag{5}$$

Reactants

Table 6: Properties of each reactant.

Id	Name	SBO
S0		
ATP		

Products

Table 7: Properties of each product.

Id	Name	SBO
S1		
Pi_		
fwd_step1		

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \mathrm{k\_1} \cdot \mathrm{S0} \cdot [\mathrm{ATP}] \cdot \exp\left(\frac{\mathrm{th\_1} \cdot \mathrm{Force} \cdot \mathrm{d}}{\mathrm{kT}}\right) \tag{6}$$

7.2 Reaction Fw_2nd_step

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

SBO:0000180 dissociation

Reaction equation

$$\mathrm{S1} \longrightarrow \mathrm{S0} + \mathrm{ADP} + \mathrm{fwd\_step2} \tag{7}$$

Reactant

Table 8: Properties of each reactant.

Id	Name	SBO
S1		

Products

Table 9: Properties of each product.

Id	Name	SBO
S0		
ADP		
fwd_step2		

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \mathrm{k\_2} \cdot \mathrm{S1} \cdot \exp\left(\frac{\mathrm{th\_2} \cdot \mathrm{Force} \cdot \mathrm{d}}{\mathrm{kT}}\right) \tag{8}$$

7.3 Reaction Bw_1st_step

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

SBO:0000376 hydrolysis

Reaction equation

$$\mathrm{S0} + \mathrm{ATP} \longrightarrow \mathrm{S1} + \mathrm{Pi\_} + \mathrm{back\_step1} \tag{9}$$

Reactants

Table 10: Properties of each reactant.

Id	Name	SBO
S0		
ATP		

Products

Table 11: Properties of each product.

Id	Name	SBO
S1		
Pi_		
back_step1		

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \text{k\_3} \cdot \text{S0} \cdot [\text{ATP}] \cdot \exp\left(\frac{\text{th\_3} \cdot \text{Force} \cdot \text{d}}{\text{kT}}\right) \tag{10}$$

7.4 Reaction Bw_2nd_step

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

SBO:0000180 dissociation

Reaction equation

$$\text{S1} \longrightarrow \text{S0} + \text{ADP} + \text{back\_step2} \tag{11}$$

Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
S1		

Products

Table 13: Properties of each product.

Id	Name	SBO
S0		
ADP		
back_step2		

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \mathrm{k\_4} \cdot \mathrm{S1} \cdot \exp\left(\frac{\mathrm{th\_4} \cdot \mathrm{Force} \cdot \mathrm{d}}{\mathrm{kT}}\right) \tag{12}$$

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.

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.

8.1 Species S0

SBO:0000297 protein complex

Initial amount 10 item

This species takes part in four reactions (as a reactant in `Fw_1st_step`, `Bw_1st_step` and as a product in `Fw_2nd_step`, `Bw_2nd_step`).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{S0} = v_2 + v_4 - v_1 - v_3 \tag{13}$$

8.2 Species ATP

SBO:0000247 simple chemical

Initial concentration 20 $\mu\mathrm{mol} \cdot \mathrm{l}^{-1}$

This species takes part in two reactions (as a reactant in `Fw_1st_step`, `Bw_1st_step`), which do not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ATP} = 0 \tag{14}$$

8.3 Species S1

SBO:0000297 protein complex

Initial amount 0 item

This species takes part in four reactions (as a reactant in Fw_2nd_step, Bw_2nd_step and as a product in Fw_1st_step, Bw_1st_step).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{S1} = v_1 + v_3 - v_2 - v_4 \tag{15}$$

8.4 Species Pi_

SBO:0000247 simple chemical

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

This species takes part in two reactions (as a product in Fw_1st_step, Bw_1st_step), which do not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Pi\_} = 0 \tag{16}$$

8.5 Species ADP

SBO:0000247 simple chemical

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

This species takes part in two reactions (as a product in Fw_2nd_step, Bw_2nd_step), which do not influence its rate of change because this species is on the boundary of the reaction system:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ADP} = 0 \tag{17}$$

8.6 Species fwd_step1

SBO:0000409 interaction outcome

Initial amount 0 item

This species takes part in one reaction (as a product in Fw_1st_step).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{fwd\_step1} = v_1 \tag{18}$$

8.7 Species fwd_step2

SBO:0000409 interaction outcome

Initial amount 0 item

This species takes part in one reaction (as a product in Fw_2nd_step).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{fwd\_step2} = v_2 \tag{19}$$

8.8 Species back_step1

SBO:0000409 interaction outcome

Initial amount 0 item

This species takes part in one reaction (as a product in Bw_1st_step).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{back\_step1} = v_3 \tag{20}$$

8.9 Species back_step2

SBO:0000409 interaction outcome

Initial amount 0 item

This species takes part in one reaction (as a product in Bw_2nd_step).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{back\_step2} = v_4 \tag{21}$$

A Glossary of Systems Biology Ontology Terms

SBO:0000022 **forward unimolecular rate constant:** Numerical parameter that quantifies the forward velocity of a chemical reaction involving only one reactant. This parameter encompasses all the contributions to the velocity except the quantity of the reactant

SBO:0000023 **forward bimolecular rate constant:** Numerical parameter that quantifies the forward velocity of a chemical reaction involving two reactants. This parameter encompasses all the contributions to the velocity except the quantity of the reactants.

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

SBO:0000247 **simple chemical:** Simple, non-repetitive chemical entity

SBO:0000290 **physical compartment:** Specific location of space, that can be bounded or not. A physical compartment can have 1, 2 or 3 dimensions

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

SBO:0000347 duration: Amount of time during which an event persists

SBO:0000360 quantity of an entity pool: The enumeration of co-localised, identical biochemical entities of a specific state, which constitute a pool. The form of enumeration may be purely numerical, or may be given in relation to another dimension such as length or volume

SBO:0000376 hydrolysis: Decomposition of a compound by reaction with water, where the hydroxyl and H groups are incorporated into different product

SBO:0000380 biochemical coefficient: number used as a multiplicative or exponential factor for quantities, expressions or function

SBO:0000409 interaction outcome: Entity that results from the interaction between other entities

SBO:0000466 length: The length of an object is the longest measurable distance between its extremities.

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.

[a]Center for Bioinformatics Tübingen (ZBIT), Germany
[b]California Institute of Technology, Beckman Institute BNMC, Pasadena, United States
[c]European Bioinformatics Institute, Wellcome Trust Genome Campus, Hinxton, United Kingdom
[d]EML Research gGmbH, Heidelberg, Germany