SBML Model Report

Model name: "Hettling2011_CreatineKinase"

May 5, 2016

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by the following two authors: Vijayalakshmi Chelliah[1] and Hannes Hettling[2] at January 26th 2012 at 1:59 p. m. and last time modified at February 25th 2015 at 12:27 a. 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	3
species types	0	species	10
events	3	constraints	0
reactions	9	function definitions	0
global parameters	57	unit definitions	5
rules	20	initial assignments	0

Model Notes

This model is from the article:
Analyzing the functional properties of the creatine kinase system with multiscale 'sloppy' modeling.
Hettling H, van Beek JH PLoS Comput Biol.2011 Aug;7(8):e1002130. PMEDID,
Abstract:

[1]EMBL-EBI, viji@ebi.ac.uk
[2]VU University Amsterdam, hettling@few.vu.nl

In this study the function of the two isoforms of creatine kinase (CK; EC 2.7.3.2) in myocardium is investigated. The 'phosphocreatine shuttle' hypothesis states that mitochondrial and cytosolic CK plays a pivotal role in the transport of high-energy phosphate (HEP) groups from mitochondria to myofibrils in contracting muscle. Temporal buffering of changes in ATP and ADP is another potential role of CK. With a mathematical model, we analyzed energy transport and damping of high peaks of ATP hydrolysis during the cardiac cycle. The analysis was based on multiscale data measured at the level of isolated enzymes, isolated mitochondria and on dynamic response times of oxidative phosphorylation measured at the whole heart level. Using 'sloppy modeling' ensemble simulations, we derived confidence intervals for predictions of the contributions by phosphocreatine (PCr) and ATP to the transfer of HEP from mitochondria to sites of ATP hydrolysis. Our calculations indicate that only 158% (meanSD) of transcytosolic energy transport is carried by PCr, contradicting the PCr shuttle hypothesis. We also predicted temporal buffering capabilities of the CK isoforms protecting against high peaks of ATP hydrolysis (3750 M*s(-1)) in myofibrils. CK inhibition by 98% in silico leads to an increase in amplitude of mitochondrial ATP synthesis pulsation from 21523 to 56631 M*s(-1), while amplitudes of oscillations in cytosolic ADP concentration double from 7711 to 1461 M. Our findings indicate that CK acts as a large bandwidth high-capacity temporal energy buffer maintaining cellular ATP homeostasis and reducing oscillations in mitochondrial metabolism. However, the contribution of CK to the transport of high-energy phosphate groups appears limited. Mitochondrial CK activity lowers cytosolic inorganic phosphate levels while cytosolic CK has the opposite effect.

2 Unit Definitions

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

2.1 Unit `micromole`

Definition $\mu\mathrm{mol}$

2.2 Unit `micromole_per_litre`

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

2.3 Unit `micromole_per_litre_per_second`

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

2.4 Unit unitDefinition_0000004

Name per_minute

Definition $(60\ \mathrm{s})^{-1}$

2.5 Unit per_second

Name per_second

Definition s^{-1}

2.6 Unit substance

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

Definition mol

2.7 Unit volume

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

Definition l

2.8 Unit area

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

Definition m^2

2.9 Unit length

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

Definition m

2.10 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
IMS	IMS		3	0.0625	l	☑	
CYT	CYT		3	0.75	l	☑	
cell	cell		3	1	litre	☑	

3.1 Compartment IMS

This is a three dimensional compartment with a constant size of 0.0625 litre.

Name IMS

3.2 Compartment CYT

This is a three dimensional compartment with a constant size of 0.75 litre.

Name CYT

3.3 Compartment cell

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

Name cell

4 Species

This model contains ten 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
ADPi	ADPi	IMS	$\mu mol \cdot l^{-1}$	⊟	⊟
ATPi	ATPi	IMS	$\mu mol \cdot l^{-1}$	⊟	⊟
Cri	Cri	IMS	$\mu mol \cdot l^{-1}$	⊟	⊟
PCri	PCri	IMS	$\mu mol \cdot l^{-1}$	⊟	⊟
PCr	PCr	CYT	$\mu mol \cdot l^{-1}$	⊟	⊟
ADP	ADP	CYT	$\mu mol \cdot l^{-1}$	⊟	⊟
ATP	ATP	CYT	$\mu mol \cdot l^{-1}$	⊟	⊟
Cr	Cr	CYT	$\mu mol \cdot l^{-1}$	⊟	⊟
P_ii	P_ii	IMS	$\mu mol \cdot l^{-1}$	⊟	⊟
P_i	P_i	CYT	$\mu mol \cdot l^{-1}$	⊟	⊟

5 Parameters

This model contains 57 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
j_diff_pcr			1.000	$\mu mol \cdot l^{-1} \cdot s^{-1}$	☐
j_diff_atp			1.000	$\mu mol \cdot l^{-1} \cdot s^{-1}$	☐
densyn			0.000		☐
tmito			0.000	s	☐
vatpnorm			0.000		☐
jsyn			0.000	$\mu mol \cdot l^{-1} \cdot s^{-1}$	☐
r_diff_pcr			1.000		☐
j_ck_mi	j_ck_mi		0.000	$\mu mol \cdot l^{-1} \cdot s^{-1}$	☐
j_ck_mm	j_ck_mm		0.000	$\mu mol \cdot l^{-1} \cdot s^{-1}$	☐
j_diff_adp			0.000	$\mu mol \cdot l^{-1} \cdot s^{-1}$	☐
j_diff_cr			0.000	$\mu mol \cdot l^{-1} \cdot s^{-1}$	☐
j_diff_pi			0.000	$\mu mol \cdot l^{-1} \cdot s^{-1}$	☐
stepsize			0.001	s	☑
phase			0.000		☐
heartrate_bpm			135.000	$(60\ s)^{-1}$	☐
heartrate_basis			135.000	$(60\ s)^{-1}$	☑
heartrate_test			220.000	$(60\ s)^{-1}$	☑
fracDia			0.667		☐
fracSysUp			0.167		☑
fracSysDown			0.167		☑
VhydAmp_basis			2918.416	$\mu mol \cdot l^{-1} \cdot s^{-1}$	☐
VhydAmp_test			3764.847	$\mu mol \cdot l^{-1} \cdot s^{-1}$	☐
time_Jhyd_step	time_Jhyd_step		40.000	s	☑
Jhyd_test	Jhyd_test		627.600	$\mu mol \cdot l^{-1} \cdot s^{-1}$	☐
Jhyd_basis	Jhyd_basis		486.500	$\mu mol \cdot l^{-1} \cdot s^{-1}$	☑
last_time_fired			0.000	s	☐
Jhyd	Jhyd		486.500	$\mu mol \cdot l^{-1} \cdot s^{-1}$	☐
ck_factor_iaa	ck_factor_iaa		1.000		☑
ck_factor_ia	ck_factor_ia		0.029		☑

Id	Name	SBO	Value	Unit	Constant
tmito_factor	tmito_factor		0.000		⊟
PSmomATP	PSmomATP		13.295	s^{-1}	☑
K_CK_eq	K_CK_eq		152.000		☑
VmaxMMb			46303.543	$\mu mol \cdot l^{-1} \cdot s^{-1}$	⊟
VmaxMib			3520.341	$\mu mol \cdot l^{-1} \cdot s^{-1}$	⊟
VmaxMif_full_activity			882.076	$\mu mol \cdot l^{-1} \cdot s^{-1}$	☑
VmaxMMf_full_activity			11441.780	$\mu mol \cdot l^{-1} \cdot s^{-1}$	☑
VmaxMif			882.076	$\mu mol \cdot l^{-1} \cdot s^{-1}$	⊟
VmaxMMf			11441.780	$\mu mol \cdot l^{-1} \cdot s^{-1}$	⊟
KiaMi			750.000	$\mu mol \cdot l^{-1}$	☑
KbMi			5200.000	$\mu mol \cdot l^{-1}$	☑
KicMi			204.800	$\mu mol \cdot l^{-1}$	☑
KdMi			500.000	$\mu mol \cdot l^{-1}$	☑
KibMi			28800.000	$\mu mol \cdot l^{-1}$	☑
KidMi			1600.000	$\mu mol \cdot l^{-1}$	☑
KiaMM			900.000	$\mu mol \cdot l^{-1}$	☑
KbMM			15500.000	$\mu mol \cdot l^{-1}$	☑
KicMM			222.400	$\mu mol \cdot l^{-1}$	☑
KdMM			1670.000	$\mu mol \cdot l^{-1}$	☑
KibMM			34900.000	$\mu mol \cdot l^{-1}$	☑
KidMM			4730.000	$\mu mol \cdot l^{-1}$	☑
Vmaxsyn	Vmaxsyn		1503.740	$\mu mol \cdot l^{-1} \cdot s^{-1}$	☑
Kadp	Kadp		25.000	$\mu mol \cdot l^{-1}$	☑
Kpi	Kpi		800.000	$\mu mol \cdot l^{-1}$	☑
PSmomPi	PSmomPi		194.000	s^{-1}	☑
PSmomCr	PSmomCr		155.000	s^{-1}	☑
PSmomPCr	PSmomPCr		155.000	s^{-1}	☑
pulsatility	pulsatility		1.000		⊟

6 Rules

This is an overview of 20 rules.

6.1 Rule `tmito`

Rule `tmito` is a rate rule for parameter `tmito`:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{tmito} = \mathrm{vatpnorm} \tag{1}$$

6.2 Rule `densyn`

Rule `densyn` is an assignment rule for parameter `densyn`:

$$\mathrm{densyn} = 1 + \frac{[\mathrm{ADPi}]}{\mathrm{Kadp}} + \frac{[\mathrm{P\_ii}]}{\mathrm{Kpi}} + \frac{[\mathrm{ADPi}] \cdot [\mathrm{P\_ii}]}{\mathrm{Kadp} \cdot \mathrm{Kpi}} \tag{2}$$

6.3 Rule `jsyn`

Rule `jsyn` is an assignment rule for parameter `jsyn`:

$$\mathrm{jsyn} = \mathrm{Vmaxsyn} \cdot \frac{[\mathrm{ADPi}] \cdot [\mathrm{P\_ii}]}{\mathrm{Kpi} \cdot \mathrm{Kadp} \cdot \mathrm{densyn}} \tag{3}$$

6.4 Rule `vatpnorm`

Rule `vatpnorm` is an assignment rule for parameter `vatpnorm`:

$$\mathrm{vatpnorm} = \mathrm{tmito\_factor} \cdot \frac{\mathrm{Jhyd\_test} - \mathrm{jsyn}}{\mathrm{Jhyd\_test} - \mathrm{Jhyd\_basis}} \tag{4}$$

6.5 Rule `VmaxMif`

Rule `VmaxMif` is an assignment rule for parameter `VmaxMif`:

$$\mathrm{VmaxMif} = \mathrm{VmaxMif\_full\_activity} \cdot \mathrm{ck\_factor\_iaa} \tag{5}$$

6.6 Rule `VmaxMMf`

Rule `VmaxMMf` is an assignment rule for parameter `VmaxMMf`:

$$\mathrm{VmaxMMf} = \mathrm{VmaxMMf\_full\_activity} \cdot \mathrm{ck\_factor\_iaa} \tag{6}$$

6.7 Rule `VmaxMib`

Rule `VmaxMib` is an assignment rule for parameter `VmaxMib`:

$$\mathrm{VmaxMib} = \frac{\mathrm{K\_CK\_eq} \cdot \mathrm{KicMi} \cdot \mathrm{KdMi} \cdot \mathrm{VmaxMif}}{\mathrm{KiaMi} \cdot \mathrm{KbMi}} \tag{7}$$

6.8 Rule VmaxMMb

Rule VmaxMMb is an assignment rule for parameter VmaxMMb:

$$\mathrm{VmaxMMb} = \frac{\mathrm{K\_CK\_eq} \cdot \mathrm{KicMM} \cdot \mathrm{KdMM} \cdot \mathrm{VmaxMMf}}{\mathrm{KiaMM} \cdot \mathrm{KbMM}} \tag{8}$$

6.9 Rule j_diff_pcr

Rule j_diff_pcr is an assignment rule for parameter j_diff_pcr:

$$\mathrm{j\_diff\_pcr} = \mathrm{PSmomPCr} \cdot (\mathrm{[PCri]} - \mathrm{[PCr]}) \tag{9}$$

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

6.10 Rule j_diff_atp

Rule j_diff_atp is an assignment rule for parameter j_diff_atp:

$$\mathrm{j\_diff\_atp} = \mathrm{PSmomATP} \cdot (\mathrm{[ATPi]} - \mathrm{[ATP]}) \tag{10}$$

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

6.11 Rule r_diff_pcr

Rule r_diff_pcr is an assignment rule for parameter r_diff_pcr:

$$\mathrm{r\_diff\_pcr} = \frac{\mathrm{j\_diff\_pcr}}{\mathrm{j\_diff\_pcr} + \mathrm{j\_diff\_atp}} \tag{11}$$

Derived unit dimensionless

6.12 Rule phase

Rule phase is an assignment rule for parameter phase:

$$\mathrm{phase} = \frac{|\mathrm{t} - \mathrm{time\_Jhyd\_step}| - \frac{\left\lfloor \frac{|\mathrm{t} - \mathrm{time\_Jhyd\_step}|}{\frac{60}{\mathrm{heartrate\_bpm}}} \right\rfloor \cdot 60}{\mathrm{heartrate\_bpm}}}{\frac{60}{\mathrm{heartrate\_bpm}}} \tag{12}$$

6.13 Rule fracDia

Rule fracDia is an assignment rule for parameter fracDia:

$$\mathrm{fracDia} = 1 - \mathrm{fracSysUp} - \mathrm{fracSysDown} \tag{13}$$

6.14 Rule VhydAmp_basis

Rule VhydAmp_basis is an assignment rule for parameter VhydAmp_basis:

$$\text{VhydAmp\_basis} = \frac{2 \cdot \text{Jhyd\_basis}}{\text{fracSysUp} + \text{fracSysDown}} \tag{14}$$

6.15 Rule VhydAmp_test

Rule VhydAmp_test is an assignment rule for parameter VhydAmp_test:

$$\text{VhydAmp\_test} = \frac{2 \cdot \text{Jhyd\_test}}{\text{fracSysUp} + \text{fracSysDown}} \tag{15}$$

6.16 Rule j_ck_mi

Rule j_ck_mi is an assignment rule for parameter j_ck_mi:

$$\text{j\_ck\_mi} \tag{16}$$
$$= \frac{\frac{\text{VmaxMif} \cdot [\text{ATPi}] \cdot [\text{Cri}]}{\text{KiaMi} \cdot \text{KbMi}} - \frac{\text{VmaxMib} \cdot [\text{ADPi}] \cdot [\text{PCri}]}{\text{KicMi} \cdot \text{KdMi}}}{1 + \frac{[\text{Cri}]}{\text{KibMi}} + \frac{[\text{PCri}]}{\text{KidMi}} + [\text{ATPi}] \cdot \left(\frac{1}{\text{KiaMi}} + \frac{[\text{Cri}]}{\text{KiaMi} \cdot \text{KbMi}} \right) + [\text{ADPi}] \cdot \left(\frac{1}{\text{KicMi}} + \frac{[\text{Cri}]}{\text{KicMi} \cdot \text{KibMi}} + \frac{[\text{PCri}]}{\text{KidMi} \cdot \frac{\text{KicMi} \cdot \text{KdMi}}{\text{KidMi}}} \right)}$$

6.17 Rule j_ck_mm

Rule j_ck_mm is an assignment rule for parameter j_ck_mm:

$$\text{j\_ck\_mm} \tag{17}$$
$$= \frac{\frac{\text{VmaxMMf} \cdot [\text{ATP}] \cdot [\text{Cr}]}{\text{KiaMM} \cdot \text{KbMM}} - \frac{\text{VmaxMMb} \cdot [\text{ADP}] \cdot [\text{PCr}]}{\text{KicMM} \cdot \text{KdMM}}}{1 + \frac{[\text{Cr}]}{\text{KibMM}} + \frac{[\text{PCr}]}{\text{KidMM}} + [\text{ATP}] \cdot \left(\frac{1}{\text{KiaMM}} + \frac{[\text{Cr}]}{\text{KiaMM} \cdot \text{KbMM}} \right) + [\text{ADP}] \cdot \left(\frac{1}{\text{KicMM}} + \frac{[\text{Cr}]}{\text{KicMM} \cdot \text{KibMM}} + \frac{[\text{PCr}]}{\text{KidMM} \cdot \frac{\text{KicMM} \cdot \text{KdMM}}{\text{KidMM}}} \right)}$$

6.18 Rule j_diff_adp

Rule j_diff_adp is an assignment rule for parameter j_diff_adp:

$$\text{j\_diff\_adp} = \text{PSmomATP} \cdot ([\text{ADPi}] - [\text{ADP}]) \tag{18}$$

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

6.19 Rule j_diff_pi

Rule j_diff_pi is an assignment rule for parameter j_diff_pi:

$$\text{j\_diff\_pi} = \text{PSmomPi} \cdot ([\text{P\_ii}] - [\text{P\_i}]) \tag{19}$$

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

6.20 Rule `j_diff_cr`

Rule `j_diff_cr` is an assignment rule for parameter `j_diff_cr`:

$$\text{j\_diff\_cr} = \text{PSmomCr} \cdot ([\text{Cri}] - [\text{Cr}]) \tag{20}$$

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

7 Events

This is an overview of three 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_0`

Name pulsatile_test

Trigger condition

$$((\text{t} \geq \text{time\_Jhyd\_step}) \wedge (\text{t} - \text{last\_time\_fired} > \text{stepsize})) \wedge (\text{pulsatility} = 1) \tag{21}$$

Delay

$$0 \tag{22}$$

Assignments

$$\text{Jhyd} = \begin{cases} \left(1 - \dfrac{\text{phase} - \text{fracSysUp}}{\text{fracSysDown}}\right) \cdot \text{VhydAmp\_test} & \text{if } (\text{phase} > \text{fracSysUp}) \wedge (\text{phase} \leq 1 - \text{fracDia}) \\ \dfrac{\text{phase}}{\text{fracSysUp}} \cdot \text{VhydAmp\_test} & \text{if phase} \leq \text{fracSysUp} \\ 0 & \text{if phase} \geq 1 - \text{fracDia} \\ \text{Jhyd} & \text{otherwise} \end{cases} \tag{23}$$

$$\text{last\_time\_fired} = \text{t} \tag{24}$$

7.2 Event `event_1`

Name pulsatile_basis

Trigger condition

$$((\text{t} < \text{time\_Jhyd\_step}) \wedge (\text{t} - \text{last\_time\_fired} \geq \text{stepsize})) \wedge (\text{pulsatility} = 1) \tag{25}$$

Delay

$$0 \tag{26}$$

Assignments

$$\text{Jhyd} = \begin{cases} 0 & \text{if phase} \leq \text{fracDia} \\ \dfrac{\text{phase} - \text{fracDia}}{\text{fracSysDown}} \cdot \text{VhydAmp\_basis} & \text{if } (\text{phase} > \text{fracDia}) \wedge (\text{phase} \leq 1 - \text{fracSysUp}) \\ \dfrac{(1 - \text{phase}) \cdot \text{VhydAmp\_basis}}{\text{fracSysUp}} & \text{if phase} > 1 - \text{fracSysUp} \\ \text{Jhyd} & \text{otherwise} \end{cases} \tag{27}$$

$$\text{last\_time\_fired} = \text{t} \tag{28}$$

7.3 Event `event_2`

Name nonpulsatile_step

Trigger condition

$$\text{t} \geq \text{time\_Jhyd\_step} \tag{29}$$

Delay

$$0 \tag{30}$$

Assignments

$$\text{Jhyd} = \begin{cases} \text{Jhyd\_test} & \text{if pulsatility} = 0 \\ \text{Jhyd} & \text{otherwise} \end{cases} \tag{31}$$

$$\text{heartrate\_bpm} = \text{heartrate\_test} \tag{32}$$

$$\text{tmito\_factor} = 1 \tag{33}$$

8 Reactions

This model contains nine 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	Jsyn		$P\_ii + ADPi \rightleftharpoons ATPi$	
2	J_CK_Mi		$ATPi + Cri \rightleftharpoons PCri + ADPi$	
3	J_CK_MM		$Cr + ATP \rightleftharpoons PCr + ADP$	
4	Jhyd_reaction		$ATP \rightleftharpoons ADP + P\_i$	
5	J_diff_Pi		$P\_ii \rightleftharpoons P\_i$	
6	J_diff_Cr		$Cri \rightleftharpoons Cr$	
7	J_diff_ADP		$ADPi \rightleftharpoons ADP$	
8	J_diff_PCr		$PCri \rightleftharpoons PCr$	
9	J_diff_ATP		$ATPi \rightleftharpoons ATP$	

8.1 Reaction Jsyn

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

Reaction equation

$$\mathrm{P\_ii} + \mathrm{ADPi} \rightleftharpoons \mathrm{ATPi} \tag{34}$$

Reactants

Table 6: Properties of each reactant.

Id	Name	SBO
P_ii	P_ii	
ADPi	ADPi	

Product

Table 7: Properties of each product.

Id	Name	SBO
ATPi	ATPi	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \frac{\mathrm{Vmaxsyn} \cdot [\mathrm{ADPi}] \cdot [\mathrm{P\_ii}]}{\mathrm{Kadp} \cdot \mathrm{Kpi} \cdot \left(1 + \frac{[\mathrm{ADPi}]}{\mathrm{Kadp}} + \frac{[\mathrm{P\_ii}]}{\mathrm{Kpi}} + \frac{[\mathrm{ADPi}] \cdot [\mathrm{P\_ii}]}{\mathrm{Kadp} \cdot \mathrm{Kpi}}\right)} \tag{35}$$

8.2 Reaction J_CK_Mi

This is a reversible reaction of two reactants forming two products.

Reaction equation

$$\mathrm{ATPi} + \mathrm{Cri} \rightleftharpoons \mathrm{PCri} + \mathrm{ADPi} \tag{36}$$

Reactants

Table 8: Properties of each reactant.

Id	Name	SBO
ATPi	ATPi	
Cri	Cri	

Products

Table 9: Properties of each product.

Id	Name	SBO
PCri	PCri	
ADPi	ADPi	

Kinetic Law

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

$$v_2 = \text{j\_ck\_mi} \tag{37}$$

8.3 Reaction J_CK_MM

This is a reversible reaction of two reactants forming two products.

Reaction equation

$$\text{Cr} + \text{ATP} \rightleftharpoons \text{PCr} + \text{ADP} \tag{38}$$

Reactants

Table 10: Properties of each reactant.

Id	Name	SBO
Cr	Cr	
ATP	ATP	

Products

Table 11: Properties of each product.

Id	Name	SBO
PCr	PCr	
ADP	ADP	

Kinetic Law

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

$$v_3 = \text{j\_ck\_mm} \tag{39}$$

8.4 Reaction Jhyd_reaction

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

Reaction equation

$$\text{ATP} \rightleftharpoons \text{ADP} + \text{P\_i} \tag{40}$$

Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
ATP	ATP	

Products

Table 13: Properties of each product.

Id	Name	SBO
ADP	ADP	
P_i	P_i	

Kinetic Law

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

$$v_4 = \text{Jhyd} \tag{41}$$

8.5 Reaction J_diff_Pi

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

Reaction equation

$$\mathrm{P\_ii} \rightleftharpoons \mathrm{P\_i} \tag{42}$$

Reactant

Table 14: Properties of each reactant.

Id	Name	SBO
P_ii	P_ii	

Product

Table 15: Properties of each product.

Id	Name	SBO
P_i	P_i	

Kinetic Law

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

$$v_5 = \mathrm{j\_diff\_pi} \tag{43}$$

8.6 Reaction J_diff_Cr

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

Reaction equation

$$\mathrm{Cri} \rightleftharpoons \mathrm{Cr} \tag{44}$$

Reactant

Table 16: Properties of each reactant.

Id	Name	SBO
Cri	Cri	

Product

Table 17: Properties of each product.

Id	Name	SBO
Cr	Cr	

Kinetic Law

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

$$v_6 = \text{j\_diff\_cr} \tag{45}$$

8.7 Reaction J_diff_ADP

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

Reaction equation

$$\text{ADPi} \rightleftharpoons \text{ADP} \tag{46}$$

Reactant

Table 18: Properties of each reactant.

Id	Name	SBO
ADPi	ADPi	

Product

Table 19: Properties of each product.

Id	Name	SBO
ADP	ADP	

Kinetic Law

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

$$v_7 = \text{j\_diff\_adp} \tag{47}$$

8.8 Reaction J_diff_PCr

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

Reaction equation

$$\mathrm{PCri} \rightleftharpoons \mathrm{PCr} \tag{48}$$

Reactant

Table 20: Properties of each reactant.

Id	Name	SBO
PCri	PCri	

Product

Table 21: Properties of each product.

Id	Name	SBO
PCr	PCr	

Kinetic Law

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

$$v_8 = \mathrm{j\_diff\_pcr} \tag{49}$$

8.9 Reaction J_diff_ATP

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

Reaction equation

$$\mathrm{ATPi} \rightleftharpoons \mathrm{ATP} \tag{50}$$

Reactant

Table 22: Properties of each reactant.

Id	Name	SBO
ATPi	ATPi	

Product

Table 23: Properties of each product.

Id	Name	SBO
ATP	ATP	

Kinetic Law

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

$$v_9 = \text{j\_diff\_atp} \tag{51}$$

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 ADPi

Name ADPi

Initial concentration $39\ \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in three reactions (as a reactant in Jsyn, J_diff_ADP and as a product in J_CK_Mi).

$$\frac{\text{d}}{\text{d}t}\text{ADPi} = v_2 - v_1 - v_7 \tag{52}$$

9.2 Species ATPi

Name ATPi

Initial concentration $5626\ \mu\text{mol} \cdot \text{l}^{-1}$

This species takes part in three reactions (as a reactant in J_CK_Mi, J_diff_ATP and as a product in Jsyn).

$$\frac{\text{d}}{\text{d}t}\text{ATPi} = v_1 - v_2 - v_9 \tag{53}$$

9.3 Species Cri

Name Cri

Initial concentration 9789 $\mu mol \cdot l^{-1}$

This species takes part in two reactions (as a reactant in J_CK_Mi, J_diff_Cr).

$$\frac{d}{dt}\text{Cri} = -v_2 - v_6 \tag{54}$$

9.4 Species PCri

Name PCri

Initial concentration 5711 $\mu mol \cdot l^{-1}$

This species takes part in two reactions (as a reactant in J_diff_PCr and as a product in J_CK_Mi).

$$\frac{d}{dt}\text{PCri} = v_2 - v_8 \tag{55}$$

9.5 Species PCr

Name PCr

Initial concentration 5710 $\mu mol \cdot l^{-1}$

This species takes part in two reactions (as a product in J_CK_MM, J_diff_PCr).

$$\frac{d}{dt}\text{PCr} = v_3 + v_8 \tag{56}$$

9.6 Species ADP

Name ADP

Initial concentration 64 $\mu mol \cdot l^{-1}$

This species takes part in three reactions (as a product in J_CK_MM, Jhyd_reaction, J_diff_ADP).

$$\frac{d}{dt}\text{ADP} = v_3 + v_4 + v_7 \tag{57}$$

9.7 Species ATP

Name ATP

Initial concentration 5601 $\mu mol \cdot l^{-1}$

This species takes part in three reactions (as a reactant in J_CK_MM, Jhyd_reaction and as a product in J_diff_ATP).

$$\frac{d}{dt}\mathrm{ATP} = v_9 - v_3 - v_4 \tag{58}$$

9.8 Species Cr

Name Cr

Initial concentration 9789 $\mu mol \cdot l^{-1}$

This species takes part in two reactions (as a reactant in J_CK_MM and as a product in J_diff_Cr).

$$\frac{d}{dt}\mathrm{Cr} = v_6 - v_3 \tag{59}$$

9.9 Species P_ii

Name P_ii

Initial concentration 910 $\mu mol \cdot l^{-1}$

This species takes part in two reactions (as a reactant in Jsyn, J_diff_Pi).

$$\frac{d}{dt}\mathrm{P\_ii} = -v_1 - v_5 \tag{60}$$

9.10 Species P_i

Name P_i

Initial concentration 912 $\mu mol \cdot l^{-1}$

This species takes part in two reactions (as a product in Jhyd_reaction, J_diff_Pi).

$$\frac{d}{dt}\mathrm{P\_i} = v_4 + v_5 \tag{61}$$

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