SBML Model Report

Model name: "Lai2007_O2_Transport_Metabolism"

May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by the following two authors: Nicola Lai[1] and Justin Chiou[2] at October 16th 2009 at 8:26 p. m. and last time modified at June third 2014 at 2:58 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	2
species types	0	species	9
events	0	constraints	0
reactions	5	function definitions	0
global parameters	50	unit definitions	7
rules	14	initial assignments	0

Model Notes

This file describes the SBML version of the mathematical model in the following journal article: Linking Pulmonary Oxygen Uptake, Muscle Oxygen Utilization and Cellular Metabolism during Exercise, Ann Biomed Eng. 2007 Jun;35(6):956-69. (Pubmed ID: 17380394). This mathematical model simulates oxygen transport and metabolism in skeletal muscle in response

[1]Case Western Reserve University, nicola.lai@case.edu
[2]Case Western Reserve University, justin.chiou@case.edu

to a step change from a warm-up steady state to a higher work rate corresponding to exercise at different levels of intensity: moderate (M), heavy (H) and very heavy (VH). The model parameter values are listed in the tables of this article. The parameter values that are independent of the exercise level are reported in Table 2. The parameter values that depend on the exercise level are reported in Tables 1A, 3 and 4. The model simulations (Figures 2, 3, 4 and 5) were obtained for a representative subject with a set of parameter values different from those in Table 1A, 3 and 4. In the sbml model, these model parameters are used to simulate exercise at a very heavy (VH) intensity for the representative subject. Additionally, the parameter values needed to simulate exercise at moderate (M) and heavy (H) intensity are reported in the list of parameters of the file. The model simulates dynamics of (1) the concentrations of free (F) and total (T) oxygen concentration in blood (CFcap, CTcap) and tissue (CFtis, CTtis), Adenosine Triphosphate (ATP), Adenosine Diphosphate (ADP), Phosphocreatine (PCr) and Creatine (Cr); (2) the metabolic flux of oxidative phosphorylation, creatine kinase and ATPase; (3) the oxygen uptake in blood and oxygen transport rate from blood to tissue during exercise. The simulation also computes muscle oxygen saturation (StO2m) and relative muscle oxygen saturation (RStO2m) in order to compare simulated and experimental responses of human muscle oxygenation during exercise. The model was successfully tested with Roadrunner of the Systems Biology Workbench (SBW). The model simulations obtained with Roadrunner match those obtained with the mathematical model represented in Fortran and Matlab for relative and absolute tolerance smaller than 10-7.

To allow for simulations at varying levels of exercise, the parameter **exercise_level** was introduced. A value of 1 means medium, 2 heavy and 3 very heavy exercise. Setting this parameter assigns the parameters **Vmax**, **KatpaseE**, **dQMm** and **tauQm** with the relevant parameters. The warmup steady state is influenced by the parameter changes for this representative subject and the model has to be brought into steady state after each change of exercise level.

2 Unit Definitions

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

2.1 Unit `substance`

Name substance

Definition mmol

2.2 Unit `perMin`

Name perMin

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

2.3 Unit `mMperMin`

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

2.4 Unit `mM`

Name mM

Definition $\mathrm{mmol} \cdot \mathrm{l}^{-1}$

2.5 Unit `time_min`

Name min

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

2.6 Unit `LperMin`

Name LperMin

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

2.7 Unit `permM`

Name permM

Definition $\mathrm{l} \cdot \mathrm{mmol}^{-1}$

2.8 Unit `volume`

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

Definition l

2.9 Unit `area`

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

Definition m^2

2.10 Unit `length`

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

Definition m

2.11 Unit `time`

Notes Second is the predefined SBML unit for `time`.

Definition s

3 Compartments

This model contains two compartments.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
`Capillary`	Capillary	0000290	3	2.0979		☑	
`Tissue`	Tissue	0000290	3	27.8721		☑	

3.1 Compartment `Capillary`

This is a three dimensional compartment with a constant size of 2.0979 litre.

Name Capillary

SBO:0000290 physical compartment

3.2 Compartment `Tissue`

This is a three dimensional compartment with a constant size of 27.8721 litre.

Name Tissue

SBO:0000290 physical compartment

4 Species

This model contains nine species. The boundary condition of two 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
ATP	ATP	Tissue	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☐
PCr	PCr	Tissue	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☐
ADP	ADP	Tissue	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☐
Cr	Cr	Tissue	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☐
Pi	Pi	Tissue	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☐
CTcap	CTcap	Capillary	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☐
CTtis	CTtis	Tissue	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☐
CFcap	CFcap	Capillary	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☑
CFtis	CFtis	Tissue	$\mathrm{mmol} \cdot \mathrm{l}^{-1}$	☐	☑

5 Parameters

This model contains 50 global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
StO2m	StO2m		0.000	dimensionless	☐
RStO2m	RStO2m		0.000	dimensionless	☐
Katpase	Katpase		0.321	$(60\,\mathrm{s})^{-1}$	☐
KatpaseW	KatpaseW		0.321	$(60\,\mathrm{s})^{-1}$	☑
Kadp	Kadp		0.058	$\mathrm{mmol}\cdot\mathrm{l}^{-1}$	☑
Kia	Kia		0.135	$\mathrm{mmol}\cdot\mathrm{l}^{-1}$	☑
Kiq	Kiq		3.500	$\mathrm{mmol}\cdot\mathrm{l}^{-1}$	☑
Kib	Kib		3.900	$\mathrm{mmol}\cdot\mathrm{l}^{-1}$	☑
Kp	Kp		3.800	$\mathrm{mmol}\cdot\mathrm{l}^{-1}$	☑
Kb	Kb		1.110	$\mathrm{mmol}\cdot\mathrm{l}^{-1}$	☑
Km	Km		$7\cdot10^{-4}$	$\mathrm{mmol}\cdot\mathrm{l}^{-1}$	☑
VfCK	VfCK		6000.000	$\mathrm{mmol}\cdot(60\,\mathrm{s})^{-1}\cdot\mathrm{l}^{-1}$	☑
VrCK	VrCK		3008.658	$\mathrm{mmol}\cdot(60\,\mathrm{s})^{-1}\cdot\mathrm{l}^{-1}$	☑
QRm	QRm		0.688	$\mathrm{l}\cdot(60\,\mathrm{s})^{-1}$	☑
QWm	QWm		3.118	$\mathrm{l}\cdot(60\,\mathrm{s})^{-1}$	☑
Qm	Qm		3.118	$\mathrm{l}\cdot(60\,\mathrm{s})^{-1}$	☐
Qc	Qc		8.000	$\mathrm{l}\cdot(60\,\mathrm{s})^{-1}$	☑
PSR	PSR		134.283	$\mathrm{l}\cdot(60\,\mathrm{s})^{-1}$	☑
PSE	PSE		20000.000	$\mathrm{l}\cdot(60\,\mathrm{s})^{-1}$	☑
PSm	PSm		5338.800	$\mathrm{l}\cdot(60\,\mathrm{s})^{-1}$	☐
nH	nH		2.700	dimensionless	☑
Hct	Hct		0.450	dimensionless	☑
Wmc			0.806	dimensionless	☑
CmcMb	CmcMb		0.500	$\mathrm{mmol}\cdot\mathrm{l}^{-1}$	☑
CrbcHb	CrbcHb		5.180	$\mathrm{mmol}\cdot\mathrm{l}^{-1}$	☑
KMb	KMb		308.642	$\mathrm{l}\cdot\mathrm{mmol}^{-1}$	☑
KHb	KHb		7800.700	$\mathrm{mmol}\cdot\mathrm{l}^{-1}$	☑
tE	tE		3.000	$(60\,\mathrm{s})^{-1}$	☑
CTart	CTart		9.200	$\mathrm{mmol}\cdot\mathrm{l}^{-1}$	☑
Vmax	Vmax		23.117	$\mathrm{mmol}\cdot(60\,\mathrm{s})^{-1}\cdot\mathrm{l}^{-1}$	☐
VmaxM	VmaxM		53.515	$\mathrm{mmol}\cdot(60\,\mathrm{s})^{-1}\cdot\mathrm{l}^{-1}$	☑

Id	Name	SBO	Value	Unit	Constant
VmaxH	VmaxH		34.687	$\mathrm{mmol} \cdot (60\,\mathrm{s})^{-1} \cdot \mathrm{l}^{-1}$	☑
VmaxVH	VmaxVH		23.117	$\mathrm{mmol} \cdot (60\,\mathrm{s})^{-1} \cdot \mathrm{l}^{-1}$	☑
KatpaseE	KatpaseE		3.342	$(60\,\mathrm{s})^{-1}$	☐
KatpaseM	KatpaseM		1.711	$(60\,\mathrm{s})^{-1}$	☑
KatpaseH	KatpaseH		2.258	$(60\,\mathrm{s})^{-1}$	☑
KatpaseVH	KatpaseVH		3.342	$(60\,\mathrm{s})^{-1}$	☑
dQMm	dQMm		12.750	$\mathrm{l} \cdot (60\,\mathrm{s})^{-1}$	☐
dQMmM	dQMmM		7.917	$\mathrm{l} \cdot (60\,\mathrm{s})^{-1}$	☑
dQMmH	dQMmH		9.422	$\mathrm{l} \cdot (60\,\mathrm{s})^{-1}$	☑
dQMmVH	dQMmVH		12.750	$\mathrm{l} \cdot (60\,\mathrm{s})^{-1}$	☑
tauQm	tauQm		0.420	$(60\,\mathrm{s})^{-1}$	☐
tauQmM	tauQmM		0.320	$(60\,\mathrm{s})^{-1}$	☑
tauQmH	tauQmH		0.396	$(60\,\mathrm{s})^{-1}$	☑
tauQmVH	tauQmVH		0.420	$(60\,\mathrm{s})^{-1}$	☑
StO2mW	StO2mW		81.171	dimensionless	☑
exercise_level	exercise_level		3.000	dimensionless	☑
ATPase_flux_mM	ATPase_flux_mM		0.000	$\mathrm{mmol} \cdot (60\,\mathrm{s})^{-1} \cdot \mathrm{l}^{-1}$	☐
CK_flux_mM	CK_flux_mM		0.000	$\mathrm{mmol} \cdot (60\,\mathrm{s})^{-1} \cdot \mathrm{l}^{-1}$	☐
oxygen_phosph	oxygen_phosphorilation_rate_mM		0.000	$\mathrm{mmol} \cdot (60\,\mathrm{s})^{-1} \cdot \mathrm{l}^{-1}$	☐

6 Rules

This is an overview of 14 rules.

6.1 Rule CFcap

Rule CFcap is a rate rule for species CFcap:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{CFcap} = \frac{(\mathrm{Qm} \cdot (\mathrm{CTart} - [\mathrm{CTcap}]) - \mathrm{PSm} \cdot ([\mathrm{CFcap}] - [\mathrm{CFtis}])) \cdot \frac{1}{\mathrm{vol}(\mathrm{Capillary})}}{1 + \frac{4 \cdot \mathrm{Hct} \cdot \mathrm{CrbcHb} \cdot \mathrm{KHb} \cdot \mathrm{nH} \cdot [\mathrm{CFcap}]^{\mathrm{nH}-1}}{(1 + \mathrm{KHb} \cdot [\mathrm{CFcap}]^{\mathrm{nH}})^2}} \tag{1}$$

6.2 Rule CFtis

Rule CFtis is a rate rule for species CFtis:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{CFtis} = \frac{\frac{\mathrm{PSm}\cdot([\mathrm{CFcap}]-[\mathrm{CFtis}])}{\mathrm{vol}(\mathrm{Tissue})} - \mathrm{Vmax}\cdot\frac{\frac{[\mathrm{CFtis}]}{\mathrm{Km}+[\mathrm{CFtis}]}\cdot[\mathrm{ADP}]}{\mathrm{Kadp}+[\mathrm{ADP}]}}{1+\frac{\mathrm{Wmc}\cdot\mathrm{CmcMb}\cdot\mathrm{KMb}}{(1+\mathrm{KMb}\cdot[\mathrm{CFtis}])^2}} \tag{2}$$

6.3 Rule Katpase

Rule Katpase is an assignment rule for parameter Katpase:

$$\mathrm{Katpase} = \begin{cases}\mathrm{KatpaseW} & \text{if time} \leq \mathrm{tE}\\ \mathrm{KatpaseE} & \text{otherwise}\end{cases} \tag{3}$$

Derived unit $(60\,\mathrm{s})^{-1}$

6.4 Rule Qm

Rule Qm is an assignment rule for parameter Qm:

$$\mathrm{Qm} = \begin{cases}\mathrm{QWm} & \text{if time} \leq \mathrm{tE}\\ \mathrm{QWm} + \mathrm{dQMm}\cdot\left(1-\exp\left(\frac{\mathrm{tE}-\mathrm{time}}{\mathrm{tauQm}}\right)\right) & \text{otherwise}\end{cases} \tag{4}$$

6.5 Rule PSm

Rule PSm is an assignment rule for parameter PSm:

$$\mathrm{PSm} = \mathrm{PSR} + (\mathrm{PSE}-\mathrm{PSR})\cdot\left(1-\exp\left(\frac{\mathrm{QRm}-\mathrm{Qm}}{\mathrm{Qc}}\right)\right) \tag{5}$$

6.6 Rule StO2m

Rule StO2m is an assignment rule for parameter StO2m:

$$\mathrm{StO2m} = \frac{100\cdot\left(\frac{\mathrm{Hct}\cdot\mathrm{CrbcHb}\cdot\mathrm{KHb}\cdot[\mathrm{CFcap}]^{\mathrm{nH}}}{1+\mathrm{KHb}\cdot[\mathrm{CFcap}]^{\mathrm{nH}}}\cdot\mathrm{vol}\,(\mathrm{Capillary}) + \frac{\mathrm{Wmc}\cdot\mathrm{CmcMb}\cdot\mathrm{KMb}\cdot[\mathrm{CFtis}]}{1+\mathrm{KMb}\cdot[\mathrm{CFtis}]}\cdot\mathrm{vol}\,(\mathrm{Tissue})\right)}{\mathrm{CrbcHb}\cdot\mathrm{Hct}\cdot\mathrm{vol}\,(\mathrm{Capillary}) + \mathrm{CmcMb}\cdot\mathrm{Wmc}\cdot\mathrm{vol}\,(\mathrm{Tissue})} \tag{6}$$

6.7 Rule RStO2m

Rule RStO2m is an assignment rule for parameter RStO2m:

$$\mathrm{RStO2m} = \frac{\mathrm{StO2m}}{\mathrm{StO2mW}} - 1 \tag{7}$$

6.8 Rule Vmax

Rule Vmax is an assignment rule for parameter Vmax:

$$\text{Vmax} = \begin{cases} \text{VmaxM} & \text{if exercise\_level} = 1 \\ \begin{cases} \text{VmaxH} & \text{if exercise\_level} = 2 \\ \text{VmaxVH} & \text{otherwise} \end{cases} & \text{otherwise} \end{cases} \tag{8}$$

Derived unit $\text{mmol} \cdot (60\ \text{s})^{-1} \cdot \text{l}^{-1}$

6.9 Rule KatpaseE

Rule KatpaseE is an assignment rule for parameter KatpaseE:

$$\text{KatpaseE} = \begin{cases} \text{KatpaseM} & \text{if exercise\_level} = 1 \\ \begin{cases} \text{KatpaseH} & \text{if exercise\_level} = 2 \\ \text{KatpaseVH} & \text{otherwise} \end{cases} & \text{otherwise} \end{cases} \tag{9}$$

Derived unit $(60\ \text{s})^{-1}$

6.10 Rule dQMm

Rule dQMm is an assignment rule for parameter dQMm:

$$\text{dQMm} = \begin{cases} \text{dQMmM} & \text{if exercise\_level} = 1 \\ \begin{cases} \text{dQMmH} & \text{if exercise\_level} = 2 \\ \text{dQMmVH} & \text{otherwise} \end{cases} & \text{otherwise} \end{cases} \tag{10}$$

Derived unit $1 \cdot (60\ \text{s})^{-1}$

6.11 Rule tauQm

Rule tauQm is an assignment rule for parameter tauQm:

$$\text{tauQm} = \begin{cases} \text{tauQmM} & \text{if exercise\_level} = 1 \\ \begin{cases} \text{tauQmH} & \text{if exercise\_level} = 2 \\ \text{tauQmVH} & \text{otherwise} \end{cases} & \text{otherwise} \end{cases} \tag{11}$$

Derived unit $(60\ \text{s})^{-1}$

6.12 Rule ATPase_flux_mM

Rule ATPase_flux_mM is an assignment rule for parameter ATPase_flux_mM:

$$\text{ATPase\_flux\_mM} = \frac{\text{ATPase}}{\text{vol}\,(\text{Tissue})} \tag{12}$$

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

6.13 Rule CK_flux_mM

Rule CK_flux_mM is an assignment rule for parameter CK_flux_mM:

$$\text{CK\_flux\_mM} = 1 \cdot \frac{\text{CreatineKinase}}{\text{vol}\left(\text{Tissue}\right)} \tag{13}$$

6.14 Rule oxygen_phosph

Rule oxygen_phosph is an assignment rule for parameter oxygen_phosph:

$$\text{oxygen\_phosph} = \frac{\text{OxidativePhosphorylation}}{\text{vol}\left(\text{Tissue}\right)} \cdot 6 \tag{14}$$

7 Reactions

This model contains five 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	`ATPase`	ATPase	$\text{ATP} \rightleftharpoons \text{ADP}$	0000376
2	`OxidativePhosphorylation`	OxidativePhosphorylation	$6\,\text{ADP} + \text{CTtis} \xrightleftharpoons{\text{Pi, CFtis}} 6\,\text{ATP}$	0000216
3	`ConvectionTransport`	ConvectionTransport	$\emptyset \rightleftharpoons \text{CTcap}$	0000185
4	`DiffusionTransport`	DiffusionTransport	$\text{CTcap} \xrightleftharpoons{\text{CFcap, CFtis}} \text{CTtis}$	0000185
5	`CreatineKinase`	CreatineKinase	$\text{ADP} + \text{PCr} \rightleftharpoons \text{ATP} + \text{Cr}$	0000216

7.1 Reaction `ATPase`

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

Name ATPase

SBO:0000376 hydrolysis

Reaction equation

$$\mathrm{ATP} \rightleftharpoons \mathrm{ADP} \tag{15}$$

Reactant

Table 6: Properties of each reactant.

Id	Name	SBO
`ATP`	ATP	

Product

Table 7: Properties of each product.

Id	Name	SBO
`ADP`	ADP	

Kinetic Law

SBO:0000049 mass action rate law for first order irreversible reactions, continuous scheme

Derived unit $(60\ \mathrm{s})^{-1} \cdot \mathrm{mmol}$

$$v_1 = \mathrm{vol}\,(\mathrm{Tissue}) \cdot \mathrm{Katpase} \cdot [\mathrm{ATP}] \tag{16}$$

7.2 Reaction `OxidativePhosphorylation`

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

Name OxidativePhosphorylation

SBO:0000216 phosphorylation

Reaction equation

$$6\,\mathrm{ADP} + \mathrm{CTtis} \xrightleftharpoons{\mathrm{Pi},\ \mathrm{CFtis}} 6\,\mathrm{ATP} \tag{17}$$

Reactants

Table 8: Properties of each reactant.

Id	Name	SBO
ADP	ADP	
CTtis	CTtis	

Modifiers

Table 9: Properties of each modifier.

Id	Name	SBO
Pi	Pi	
CFtis	CFtis	

Product

Table 10: Properties of each product.

Id	Name	SBO
ATP	ATP	

Kinetic Law

SBO:0000432 irreversible Michaelis Menten rate law for two substrates

Derived unit $0.0010\ \mathrm{mol} \cdot (60\ \mathrm{s})^{-1}$

$$v_2 = \frac{\mathrm{vol}\left(\mathrm{Tissue}\right) \cdot \mathrm{Vmax} \cdot \frac{[\mathrm{CFtis}]}{\mathrm{Km}+[\mathrm{CFtis}]} \cdot [\mathrm{ADP}]}{\mathrm{Kadp} + [\mathrm{ADP}]} \tag{18}$$

7.3 Reaction ConvectionTransport

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

Name ConvectionTransport

SBO:0000185 transport reaction

Reaction equation

$$\emptyset \rightleftharpoons \mathrm{CTcap} \tag{19}$$

Product

Table 11: Properties of each product.

Id	Name	SBO
CTcap	CTcap	

Kinetic Law

Derived unit $(60\,\mathrm{s})^{-1} \cdot \mathrm{mmol}$

$$v_3 = \mathrm{Qm} \cdot (\mathrm{CTart} - [\mathrm{CTcap}]) \tag{20}$$

7.4 Reaction `DiffusionTransport`

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

Name DiffusionTransport

SBO:0000185 transport reaction

Reaction equation

$$\mathrm{CTcap} \xrightleftharpoons{\mathrm{CFcap},\ \mathrm{CFtis}} \mathrm{CTtis} \tag{21}$$

Reactant

Table 12: Properties of each reactant.

Id	Name	SBO
CTcap	CTcap	

Modifiers

Table 13: Properties of each modifier.

Id	Name	SBO
CFcap	CFcap	
CFtis	CFtis	

Product

Table 14: Properties of each product.

Id	Name	SBO
CTtis	CTtis	

Kinetic Law

Derived unit $(60\ \mathrm{s})^{-1} \cdot \mathrm{mmol}$

$$v_4 = \mathrm{PSm} \cdot ([\mathrm{CFcap}] - [\mathrm{CFtis}]) \tag{22}$$

7.5 Reaction `CreatineKinase`

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

Name CreatineKinase

SBO:0000216 phosphorylation

Reaction equation

$$\mathrm{ADP} + \mathrm{PCr} \rightleftharpoons \mathrm{ATP} + \mathrm{Cr} \tag{23}$$

Reactants

Table 15: Properties of each reactant.

Id	Name	SBO
ADP	ADP	
PCr	PCr	

Products

Table 16: Properties of each product.

Id	Name	SBO
ATP	ATP	
Cr	Cr	

Kinetic Law

Derived unit $0.0010000000000000013\ \mathrm{mol} \cdot (60\ \mathrm{s})^{-1}$

$$v_5 = \frac{\mathrm{vol}\left(\mathrm{Tissue}\right) \cdot \left(\frac{\mathrm{VfCK} \cdot [\mathrm{ADP}] \cdot [\mathrm{PCr}]}{\mathrm{Kb} \cdot \mathrm{Kia}} - \frac{\mathrm{VrCK} \cdot [\mathrm{Cr}] \cdot [\mathrm{ATP}]}{\mathrm{Kiq} \cdot \mathrm{Kp}}\right)}{\frac{\mathrm{Kia} + [\mathrm{ADP}]}{\mathrm{Kia}} + \frac{[\mathrm{ATP}]}{\mathrm{Kiq}} + \frac{[\mathrm{PCr}]}{\mathrm{Kib}} + \frac{[\mathrm{ADP}] \cdot [\mathrm{PCr}]}{\mathrm{Kb} \cdot \mathrm{Kia}} + \frac{[\mathrm{Cr}] \cdot [\mathrm{ATP}]}{\mathrm{Kiq} \cdot \mathrm{Kp}}} \quad (24)$$

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.

8.1 Species ATP

Name ATP

SBO:0000247 simple chemical

Initial concentration $8.198857 \mathrm{mmol} \cdot \mathrm{l}^{-1}$

This species takes part in three reactions (as a reactant in ATPase and as a product in OxidativePhosphorylation, CreatineKinase).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ATP} = 6v_2 + v_5 - v_1 \quad (25)$$

8.2 Species PCr

Name PCr

SBO:0000247 simple chemical

Initial concentration $40.98942 \mathrm{mmol} \cdot \mathrm{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{PCr} = -v_5 \quad (26)$$

8.3 Species ADP

Name ADP

SBO:0000247 simple chemical

Initial concentration $0.001142 \mathrm{mmol} \cdot \mathrm{l}^{-1}$

This species takes part in three reactions (as a reactant in OxidativePhosphorylation, CreatineKinase and as a product in ATPase).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{ADP} = v_1 - 6v_2 - v_5 \quad (27)$$

8.4 Species Cr

Name Cr

SBO:0000247 simple chemical

Initial concentration $1.01056 \text{ mmol} \cdot \text{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Cr} = v_5 \tag{28}$$

8.5 Species Pi

Name Pi

SBO:0000247 simple chemical

Initial concentration $0.5 \text{ mmol} \cdot \text{l}^{-1}$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Pi} = 0 \tag{29}$$

8.6 Species CTcap

Name CTcap

SBO:0000247 simple chemical

Initial concentration $5.281527 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a reactant in DiffusionTransport and as a product in ConvectionTransport).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{CTcap} = v_3 - v_4 \tag{30}$$

8.7 Species CTtis

Name CTtis

SBO:0000247 simple chemical

Initial concentration $0.4084824 \text{ mmol} \cdot \text{l}^{-1}$

This species takes part in two reactions (as a reactant in OxidativePhosphorylation and as a product in DiffusionTransport).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{CTtis} = v_4 - v_2 \tag{31}$$

8.8 Species CFcap

Name CFcap

SBO:0000247 simple chemical

Initial concentration $0.03969 \text{ mmol} \cdot \text{l}^{-1}$

Involved in rule CFcap

This species takes part in one reaction (as a modifier in DiffusionTransport). Not this but one rule determines the species' quantity because this species is on the boundary of the reaction system.

8.9 Species CFtis

Name CFtis

SBO:0000247 simple chemical

Initial concentration $0.0374 \text{ mmol} \cdot \text{l}^{-1}$

Involved in rule CFtis

This species takes part in two reactions (as a modifier in OxidativePhosphorylation, DiffusionTransport). Not these but one rule determines the species' quantity because this species is on the boundary of the reaction system.

A Glossary of Systems Biology Ontology Terms

SBO:0000049 mass action rate law for first order irreversible reactions, continuous scheme: Reaction scheme where the products are created from the reactants and the change of a product quantity is proportional to the product of reactant activities. The reaction scheme does not include any reverse process that creates the reactants from the products. The change of a product quantity is proportional to the quantity of one reactant. It is to be used in a reaction modelled using a continuous framework.

SBO:0000185 transport reaction: Movement of a physical entity without modification of the structure of the entity

SBO:0000216 phosphorylation: Addition of a phosphate group (-H2PO4) to a chemical entity

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

SBO:0000432 irreversible Michaelis Menten rate law for two substrates: Enzymatic rate law for an irreversible reaction involving two substrates and one product.

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