SBML Model Report

Model name:
“vanBeek2007_OxPhos_HeartMuscleCells”

May 6, 2016

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by the following three authors: Catherine Lloyd¹, Catherine Lloyd² and Catherine Lloyd³ at June 25th 2010 at 12:35 a.m. and last time modified at June 25th 2010 at 12:35 a.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.

<table>
<thead>
<tr>
<th>Element</th>
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<th>Element</th>
<th>Quantity</th>
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<td>32</td>
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</tr>
</tbody>
</table>

Model Notes

This a model from the article:
Adenine nucleotide-creatine-phosphate module in myocardial metabolic system explains fast phase of dynamic regulation of oxidative phosphorylation.

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van Beek JH. Am J Physiol Cell Physiol 2007 Sep;293(3):C815-29 17581855 ,

Abstract:
Computational models of a large metabolic system can be assembled from modules that represent a biological function emerging from interaction of a small subset of molecules. A "skeleton model," is tested here for a module that regulates the first phase of dynamic adaptation of oxidative phosphorylation (OxPhos) to demand in heart muscle cells. The model contains only diffusion, mitochondrial outer membrane (MOM) permeation, and two isoforms of creatine kinase (CK), cytosol and mitochondrial intermembrane space (IMS), respectively. The communication with two neighboring modules occurs via stimulation of mitochondrial ATP production by ADP and P(i) from the IMS and via time-varying cytosolic ATP hydrolysis during contraction. Assuming normal cytosolic diffusion and high MOM permeability for ADP, the response time of OxPhos (t(mito); generalized time constant) to steps in cardiac pacing rate is predicted to be 2.4 s. In contrast, with low MOM permeability, t(mito) is predicted to be 15 s. An optimized MOM permeability of 21 mum/s gives t(mito) = 3.7 s, in agreement with experiments on rabbit heart with blocked glycolytic ATP synthesis. The model correctly predicts a lower t(mito) if CK activity is reduced by 98%. Among others, the following predictions result from the model analysis: 1) CK activity buffers large ADP oscillations; 2) ATP production is pulsatile in beating heart, although it adapts slowly to demand with a time constant, approximately 14 heartbeats; 3) if the muscle isoform of CK is overexpressed, OxPhos reacts slower to changing workload; and 4) if mitochondrial CK is overexpressed, OxPhos reacts faster.

This model was taken from the CellML repository and automatically converted to SBML. The original model was: van Beek JH. (2007) - version=1.0
The original CellML model was created by:
Catherine Lloyd
c.lloyd@auckland.ac.nz
The University of Auckland

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2 Unit Definitions

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

2.1 Unit micromolar
Name micromolar
Definition $\mu\text{mol}\cdot\text{l}^{-1}$

2.2 Unit flux
Name flux
Definition $\mu\text{mol}\cdot\text{l}^{-1}\cdot\text{s}^{-1}$

2.3 Unit first_order_rate_constant
Name first_order_rate_constant
Definition $\text{s}^{-1}$

2.4 Unit substance
Notes Mole is the predefined SBML unit for substance.
Definition mol

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.

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<th>Id</th>
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<th>Unit</th>
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</table>

3.1 Compartment COMpartment

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

4 Parameters

This model contains 63 global parameters.

Table 3: Properties of each parameter.

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<tr>
<th>Id</th>
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<th>Value</th>
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<th>Constant</th>
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</table>
5 Rules

This is an overview of 32 rules.

5.1 Rule ATP\_cyt

Rule ATP\_cyt is a rate rule for parameter ATP\_cyt:

\[
\frac{d}{dt} \text{ATP\_cyt} = \frac{J_{\text{diff\_ATP}} - (J_{\text{hyd}} + J_{\text{CKMM}})}{V_{\text{cyt}}}\]

(1)

5.2 Rule ADP\_cyt

Rule ADP\_cyt is a rate rule for parameter ADP\_cyt:

\[
\frac{d}{dt} \text{ADP\_cyt} = \frac{J_{\text{diff\_ADP}} + J_{\text{hyd}} + J_{\text{CKMM}}}{V_{\text{cyt}}}\]

(2)

5.3 Rule PCr\_cyt

Rule PCr\_cyt is a rate rule for parameter PCr\_cyt:

\[
\frac{d}{dt} \text{PCr\_cyt} = \frac{J_{\text{diff\_PCr}} + J_{\text{CKMM}}}{V_{\text{cyt}}}\]

(3)

5.4 Rule Cr\_cyt

Rule Cr\_cyt is a rate rule for parameter Cr\_cyt:

\[
\frac{d}{dt} \text{Cr\_cyt} = \frac{J_{\text{diff\_Cr}} - J_{\text{CKMM}}}{V_{\text{cyt}}}\]

(4)

5.5 Rule Pi\_cyt

Rule Pi\_cyt is a rate rule for parameter Pi\_cyt:

\[
\frac{d}{dt} \text{Pi\_cyt} = \frac{J_{\text{diff\_Pi}} + J_{\text{hyd}}}{V_{\text{cyt}}}\]

(5)
5.6 Rule ATP_ims

Rule ATP_ims is a rate rule for parameter ATP_ims:

\[
\frac{d}{dt} \text{ATP}_\text{ims} = \frac{J_{\text{syn}} - (J_{\text{diff,ATP}} + J_{\text{CKM}_\text{im}})}{V_{\text{ims}}} \quad (6)
\]

5.7 Rule ADP_ims

Rule ADP_ims is a rate rule for parameter ADP_ims:

\[
\frac{d}{dt} \text{ADP}_\text{ims} = \frac{J_{\text{CKM}_\text{im}} - (J_{\text{syn}} + J_{\text{diff,ADP}})}{V_{\text{ims}}} \quad (7)
\]

5.8 Rule PCr_ims

Rule PCr_ims is a rate rule for parameter PCr_ims:

\[
\frac{d}{dt} \text{PCr}_\text{ims} = \frac{J_{\text{CKM}_\text{im}} - J_{\text{diff,PCr}}}{V_{\text{ims}}} \quad (8)
\]

5.9 Rule Cr_ims

Rule Cr_ims is a rate rule for parameter Cr_ims:

\[
\frac{d}{dt} \text{Cr}_\text{ims} = \frac{(J_{\text{CKM}_\text{im}} + J_{\text{diff,Cr}})}{V_{\text{ims}}} \quad (9)
\]

5.10 Rule Pi_ims

Rule Pi_ims is a rate rule for parameter Pi_ims:

\[
\frac{d}{dt} \text{Pi}_\text{ims} = \frac{(J_{\text{syn}} + J_{\text{diff,Pi}})}{V_{\text{ims}}} \quad (10)
\]

5.11 Rule J_CKMM

Rule J_CKMM is an assignment rule for parameter J_CKMM:

\[
J_{\text{CKMM}} = \frac{V_{\text{max,MM}_f} \cdot \frac{\text{ATP}_\text{c}_\text{y} \cdot \text{Cr}_\text{c}_\text{y}}{K_{\text{a}_{\text{MM},\text{CKM}}} K_{b} J_{\text{CKM}}}}{V_{\text{max,MM}_b} \cdot \frac{\text{ADP}_\text{c}_\text{y} \cdot \text{PCr}_\text{c}_\text{y}}{K_{c} J_{\text{CKMM}} K_{d} J_{\text{CKMM}}}} \quad \text{Den}_{\text{MMCK}} \quad (11)
\]

Produced by S\textsc{BML}2\textsc{TEX}
5.12 Rule Den_MMCK

Rule Den_MMCK is an assignment rule for parameter Den_MMCK:

\[
Den_{\text{MMCK}} = 1 + \frac{\text{Cr}_{\text{cyt}}}{\text{Kib}_{\text{JCKMM}}} + \frac{\text{PCr}_{\text{cyt}}}{\text{Kid}_{\text{JCKMM}}} + \text{ATP}_{\text{cyt}} \cdot \left(\frac{1}{\text{Kia}_{\text{JCKMM}}} + \frac{\text{Cr}_{\text{cyt}}}{\text{Kia}_{\text{JCKMM}} \cdot \text{Kb}_{\text{JCKMM}}}\right) \\
+ \text{ADP}_{\text{cyt}} \cdot \left(\frac{1}{\text{Kic}_{\text{JCKMM}}} + \frac{\text{PCr}_{\text{cyt}}}{\text{Kid}_{\text{JCKMM}} \cdot \text{Kc}_{\text{JCKMM}}} + \frac{\text{Cr}_{\text{cyt}}}{\text{Kic}_{\text{JCKMM}} \cdot \text{KIb}_{\text{JCKMM}}}\right)
\]  

(12)

5.13 Rule Kc_J_CKMM

Rule Kc_J_CKMM is an assignment rule for parameter Kc_J_CKMM:

\[
Kc_{\text{JCKMM}} = \frac{\text{Kic}_{\text{JCKMM}} \cdot \text{Kd}_{\text{JCKMM}}}{\text{Kid}_{\text{JCKMM}}}
\]  

(13)

5.14 Rule KIb_J_CKMM

Rule KIb_J_CKMM is an assignment rule for parameter KIb_J_CKMM:

\[
\text{KIB}_{\text{JCKMM}} = \text{KIB}_{\text{JCKMM}}
\]  

(14)

5.15 Rule J_CKMi

Rule J_CKMi is an assignment rule for parameter J_CKMi:

\[
J_{\text{CKMi}} = \frac{\text{Vmax}_{\text{Mi,f}} \cdot \text{ATP}_{\text{ims}} \cdot \text{Cr}_{\text{ims}}}{\text{Kia}_{\text{JCKMi}} \cdot \text{Ki}_{\text{CKMi}} \cdot \text{Kb}_{\text{JCKMi}}} - \frac{\text{Vmax}_{\text{Mi,b}} \cdot \text{ADP}_{\text{ims}} \cdot \text{PCr}_{\text{ims}}}{\text{Kic}_{\text{JCKMi}} \cdot \text{Kd}_{\text{JCKMi}}}
\]  

(15)

5.16 Rule Den_MiCK

Rule Den_MiCK is an assignment rule for parameter Den_MiCK:

\[
Den_{\text{MiCK}} = 1 + \frac{\text{Cr}_{\text{ims}}}{\text{Kib}_{\text{JCKMi}}} + \frac{\text{PCr}_{\text{ims}}}{\text{Kid}_{\text{JCKMi}}} + \text{ATP}_{\text{ims}} \cdot \left(\frac{1}{\text{Kia}_{\text{JCKMi}}} + \frac{\text{Cr}_{\text{ims}}}{\text{Kia}_{\text{JCKMi}} \cdot \text{Kb}_{\text{JCKMi}}}\right) + \text{ADP}_{\text{ims}} \cdot \left(\frac{1}{\text{Kic}_{\text{JCKMi}}} + \frac{\text{PCr}_{\text{ims}}}{\text{Kid}_{\text{JCKMi}} \cdot \text{Kc}_{\text{JCKMi}}} + \frac{\text{Cr}_{\text{ims}}}{\text{Kic}_{\text{JCKMi}} \cdot \text{KIb}_{\text{JCKMi}}}\right)
\]  

(16)
5.17 Rule $K_{c, J, CKMi}$

Rule $K_{c, J, CKMi}$ is an assignment rule for parameter $K_{c, J, CKMi}$:

$$K_{c, J, CKMi} = \frac{K_{ic, J, CKMi} \cdot K_{d, J, CKMi}}{K_{id, J, CKMi}}$$

(17)

5.18 Rule $K_{ib, J, CKMi}$

Rule $K_{ib, J, CKMi}$ is an assignment rule for parameter $K_{ib, J, CKMi}$:

$$K_{ib, J, CKMi} = K_{ib, J, CKMi}$$

(18)

5.19 Rule $t_{cycle_1}$

Rule $t_{cycle_1}$ is an assignment rule for parameter $t_{cycle_1}$:

$$t_{cycle_1} = \frac{60}{freq_1}$$

(19)

5.20 Rule $t_{cycle_2}$

Rule $t_{cycle_2}$ is an assignment rule for parameter $t_{cycle_2}$:

$$t_{cycle_2} = \frac{60}{freq_2}$$

(20)

5.21 Rule $duration_1$

Rule $duration_1$ is an assignment rule for parameter $duration_1$:

$$duration_1 = nb_{of\_cycles_1} \cdot t_{cycle_1}$$

(21)

5.22 Rule $ltime$

Rule $ltime$ is an assignment rule for parameter $ltime$:

$$ltime = \begin{cases} 
\text{time} - t_{cycle_1} \cdot \left\lfloor \frac{\text{time}}{t_{cycle_1}} \right\rfloor & \text{if } \text{time} \leq duration_1 \\
\text{time} - duration_1 - t_{cycle_2} \cdot \left\lfloor \frac{\text{time} - duration_1}{t_{cycle_2}} \right\rfloor & \text{otherwise}
\end{cases}$$

(22)

5.23 Rule $t_{cycle}$

Rule $t_{cycle}$ is an assignment rule for parameter $t_{cycle}$:

$$t_{cycle} = \begin{cases} 
t_{cycle_1} & \text{if } \text{time} \leq duration_1 \\
t_{cycle_2} & \text{otherwise}
\end{cases}$$

(23)
5.24 Rule $H_{\text{ATPmax}}$

Rule $H_{\text{ATPmax}}$ is an assignment rule for parameter $H_{\text{ATPmax}}$:

$$H_{\text{ATPmax}} = \begin{cases} 
6 \cdot J_{\text{hyd, basis, 1}} & \text{if time} \leq \text{duration, 1} \\
6 \cdot J_{\text{hyd, basis, 2}} & \text{otherwise}
\end{cases}$$

(24)

5.25 Rule $J_{\text{hyd}}$

Rule $J_{\text{hyd}}$ is an assignment rule for parameter $J_{\text{hyd}}$:

$$J_{\text{hyd}} = \begin{cases} 
\frac{H_{\text{ATPmax}} \cdot \text{lt ime}}{t_{\text{cycle}}} \cdot 6 & \text{if } (\text{lt ime} \geq 0) \land (\text{lt ime} < \frac{1}{6} \cdot t_{\text{cycle}}) \\
H_{\text{ATPmax}} \cdot \left(1 - 6 \cdot \left(\frac{\text{lt ime}}{t_{\text{cycle}}} - \frac{1}{6}\right)\right) & \text{if } (\text{lt ime} \geq \frac{1}{6} \cdot t_{\text{cycle}}) \land (\text{lt ime} < \frac{1}{3} \cdot t_{\text{cycle}}) \\
0 & \text{if } (\text{lt ime} \geq \frac{1}{3} \cdot t_{\text{cycle}}) \land (\text{lt ime} < t_{\text{cycle}})
\end{cases}$$

(25)

5.26 Rule $J_{\text{syn}}$

Rule $J_{\text{syn}}$ is an assignment rule for parameter $J_{\text{syn}}$:

$$J_{\text{syn}} = V_{\text{max, syn}} \cdot \frac{ADP_{\text{ims}} \cdot Pi_{\text{ims}}}{KPi \cdot KADP \cdot Den_{\text{syn}}}$$

(26)

5.27 Rule $Den_{\text{syn}}$

Rule $Den_{\text{syn}}$ is an assignment rule for parameter $Den_{\text{syn}}$:

$$Den_{\text{syn}} = 1 + \frac{ADP_{\text{ims}}}{KADP} + \frac{Pi_{\text{ims}}}{KPi} + \frac{ADP_{\text{ims}} \cdot Pi_{\text{ims}}}{KADP \cdot KPi}$$

(27)

5.28 Rule $J_{\text{diff, ATP}}$

Rule $J_{\text{diff, ATP}}$ is an assignment rule for parameter $J_{\text{diff, ATP}}$:

$$J_{\text{diff, ATP}} = PS_{\text{tot, ATP}} \cdot (ATP_{\text{ims}} - ATP_{\text{cyt}})$$

(28)

5.29 Rule $J_{\text{diff, ADP}}$

Rule $J_{\text{diff, ADP}}$ is an assignment rule for parameter $J_{\text{diff, ADP}}$:

$$J_{\text{diff, ADP}} = PS_{\text{tot, ADP}} \cdot (ADP_{\text{ims}} - ADP_{\text{cyt}})$$

(29)

5.30 Rule $J_{\text{diff, PCr}}$

Rule $J_{\text{diff, PCr}}$ is an assignment rule for parameter $J_{\text{diff, PCr}}$:

$$J_{\text{diff, PCr}} = PS_{\text{tot, PCr}} \cdot (PCr_{\text{ims}} - PCr_{\text{cyt}})$$

(30)
5.31 Rule $J_{\text{diff}, \text{Cr}}$

Rule $J_{\text{diff}, \text{Cr}}$ is an assignment rule for parameter $J_{\text{diff}, \text{Cr}}$:

$$J_{\text{diff}, \text{Cr}} = P_{\text{tot}, \text{Cr}} \cdot (\text{Cr}_{\text{ims}} - \text{Cr}_{\text{cyt}}) \quad (31)$$

5.32 Rule $J_{\text{diff}, \text{Pi}}$

Rule $J_{\text{diff}, \text{Pi}}$ is an assignment rule for parameter $J_{\text{diff}, \text{Pi}}$:

$$J_{\text{diff}, \text{Pi}} = P_{\text{tot}, \text{Pi}} \cdot (\text{Pi}_{\text{ims}} - \text{Pi}_{\text{cyt}}) \quad (32)$$