This is Appendix describing the reaction-diffusion model of energy transfer which appeared with several typing errors in

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The correct Appendix should read as following.
Please inform us if you find any typing errors in this version.

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Appendix

Here we give the description of the mathematical models used above. Depending on dimensions, we call these 2D and 0D models. The 2D model is a continuous version of the discrete 1D model (1) obtained by adding the longitudinal dimension. This is a system of partial differential equations involving two spatial coordinates and time. Assuming the spatial homogeneity of the metabolites within the myocyte, i.e., the infinitely fast diffusion, the 2D model is simplified to a system of ordinary differential equations involving only time-dependence, hence the name 0D model. The values of the parameters used in the models are listed in Table 1.

Two-dimensional model

The dynamics of the metabolites in the myofibril and myoplasm are described by the following system of reaction-diffusion equations:

$$\frac{\partial ATP}{\partial t} = D_{ATP}\nabla^2 ATP - G_{CK}v_{CK} + G_{AK}v_{AK} - G_H H_{ATP}(t), \quad (1)$$

$$\frac{\partial ADP}{\partial t} = D_{ADP}\nabla^2 ADP + G_{CK}v_{CK} - 2G_{AK}v_{AK} + G_H H_{ATP}(t), \quad (2)$$

$$\frac{\partial AMP}{\partial t} = D_{AMP}\nabla^2 AMP + G_{AK}v_{AK}, \quad (3)$$

$$\frac{\partial PCr}{\partial t} = D_{PCr}\nabla^2 PCr + G_{CK}v_{CK}, \quad (4)$$

$$\frac{\partial Cr}{\partial t} = D_{Cr}\nabla^2 Cr - G_{CK}v_{CK}, \quad (5)$$

$$\frac{\partial Pi}{\partial t} = D_{Pi}\nabla^2 Pi + G_H H_{ATP}(t), \quad (6)$$

where ATP, ADP, AMP, PCr, Cr, Pi are the total concentrations of the metabolites in the myofibril and myoplasm, D_{Met} is the diffusion coefficient of the metabolite Met (ATP, ADP, AMP, PCr, Cr, or Pi), v_{CK} is creatine kinase (CK) reaction rate, v_{AK} is adenylate kinase (AK) reaction rate, and H_{ATP} is the rate of the ATP hydrolysis in the myofibril. The factors G_{CK}, G_{AK} and G_H describe the spatial inhomogeneities of myofibrillar CK, AK and ATPase, respectively. The symbol ∇^2 denotes the Laplace operator.

The CK reaction rate v_{CK} is described by the eq. (31),

$$v_{CK} = \left(V_1 \frac{mATP \cdot Cr}{K_{ia} K_b} - V_{-1} \frac{mADP \cdot PCr}{K_{ic} K_d} \right) / DenCK, \tag{7}$$

where

$$\begin{aligned} DenCK &= 1 + \frac{Cr}{K_{ib}} + \frac{PCr}{K_{id}} + mATP \left(\frac{1}{K_{ia}} + \frac{Cr}{K_{ia} K_b} \right) \\ &\quad + mADP \left(\frac{1}{K_{ic}} + \frac{PCr}{K_{id} K_c} + \frac{Cr}{K_{ic} K_{Ib}} \right) \end{aligned} \tag{8}$$

and

$$K_c = K_{ic} K_d / K_{id}. \tag{9}$$

The concentrations of the magnesium-bound forms of ATP and ADP are denoted by $mATP$ or $mADP$, respectively. Similarly, the magnesium-free forms are denoted by $fATP$ and $fADP$. The total concentrations of adenylates and their magnesium-bound forms are related as follows

$$fATP = \frac{ATP}{1 + Mg/K_{DT}}, \tag{10}$$

$$mATP = ATP - fATP, \tag{11}$$

$$fADP = \frac{ADP}{1 + Mg/K_{DD}}, \tag{12}$$

$$mADP = ADP - fADP. \tag{13}$$

Here Mg is the level of free magnesium, and K_{DT} and K_{DD} are magnesium dissociation constants. The level of free magnesium and its dissociation constant for matrix differ from their correspondig values for the rest of the cell (21). The reaction rate v_{AK} is described by the equation

$$v_{AK} = k_{fa} \cdot fADP \cdot mADP - k_{ba} \cdot mATP \cdot AMP \tag{14}$$

Here k_{fa} and k_{ba} are the forward and backward reaction rate constants for the AK reaction.

In this paper we approximate the hydrolysis rate by a piecewise linear time-periodic function H_{ATP}. The rate increases from 0 to $H_{ATP(max)}$ during the first 30ms, decreases to 0 during the next 30ms and remains 0 until the end of cardiac cycle at 180ms;

$$H_{ATP} = H_{ATP(base)} + \begin{cases} \frac{t}{30.0} H_{ATP(max)}, & \text{if } 0 \le t < 30 \\ \frac{60.0 - t}{30.0} H_{ATP(max)}, & \text{if } 30 \le t < 60 \\ 0.0, & \text{if } 60 \le t < 180 \end{cases}, \tag{15}$$

where t is elapsed time from the beginning of cycle, measured in ms.

The reaction rates of CK, AK and ATPase are proportional to the concentrations of the corresponding enzymes. The spatial distribution of CK (37) is described by

$$G_{CK}(x, y) = \begin{cases} 0.94(1 - \frac{x}{0.375}), & \text{if } x < 0.375 \text{ and } y < 1 \\ 1.61 \frac{x - 0.375}{0.375}, & \text{if } 0.375 \le x < 0.75 \text{ and } y < 1 \\ 1.61, & \text{if } x \ge 0.75 \text{ or } y \ge 1 \end{cases}, \tag{16}$$

the distribution of AK by

$$G_{AK}(x, y) = G_{CK}(x, y), \tag{17}$$

and that of the ATPase (3) by

$$G_H(x,y) = \begin{cases} \frac{4}{3}\frac{x}{0.125}, & \text{if } x < 0.125 \text{ and } y < 1 \\ \frac{4}{3}, & \text{if } 0.125 \le x < 0.75 \text{ and } y < 1 \\ \frac{4}{3}(1 - \frac{x-0.75}{0.125}), & \text{if } 0.75 \le x < 0.875 \text{ and } y < 1 \\ 0, & \text{if } x \ge 0.875 \text{ or } y \ge 1 \end{cases}, \tag{18}$$

where x and y are spatial coordinates measured in μm, x corresponds to the longitudinal direction (increases from M line to Z line), y corresponds to the transverse direction (increases from the myofibril core to the mitochondrion); the point with coordinates (0,0) is located at the myofibril core and M line. The mean values of G_{CK} and G_{AK} over the myofibril and myoplasm ($0 \le x \le 1$, $0 \le y \le 1.2$) and G_H over the myoplasm ($0 \le x \le 1$, $0 \le y \le 1$) are equal to unity.

Due to the symmetry of the problem, we use no flux condition at the boundaries $x = 0$, $x = 1$, and $y = 0$. The restricted diffusion through the mitochondrial outer membrane takes place at the boundary $y = 1.2$ and is calculated by

$$D_{ATP}\frac{\partial ATP}{\partial \vec{n}} = R_{ATP}(ATP_i - ATP), \tag{19}$$

$$D_{ADP}\frac{\partial ADP}{\partial \vec{n}} = R_{ADP}(ADP_i - ADP), \tag{20}$$

$$D_{AMP}\frac{\partial AMP}{\partial \vec{n}} = R_{AMP}(AMP_i - AMP), \tag{21}$$

$$D_{PCr}\frac{\partial PCr}{\partial \vec{n}} = R_{PCr}(PCr_i - PCr), \tag{22}$$

$$D_{Cr}\frac{\partial Cr}{\partial \vec{n}} = R_{Cr}(Cr_i - Cr), \tag{23}$$

$$D_{Pi}\frac{\partial Pi}{\partial \vec{n}} = R_{Pi}(Pi_i - Pi), \tag{24}$$

where Met_i is the concentration of the metabolite Met in the mitochondrial intermembrane space, and R_{Met} is the permeability of the mitochondrial outer membrane.

The concentrations of the metabolites in the intermembrane space are changed due to the diffusion through the outer membrane, CK and AK reactions, ATP/ADP translocation and Pi transportation through the inner membrane according to the following equations

$$\frac{dATP_i}{dt} = \frac{R_{ATP}}{L_i}(ATP - ATP_i) + v_{ANT}/FV_i - v_{MiCK}/FV_i + v_{AKmit}/FV_i \tag{25}$$

$$\frac{dADP_i}{dt} = \frac{R_{ADP}}{L_i}(ADP - ADP_i) - 2v_{AKmit}/FV_i - v_{ANT}/FV_i + v_{MiCK}/FV_i \tag{26}$$

$$\frac{dAMP_i}{dt} = \frac{R_{AMP}}{L_i}(AMP - AMP_i) + v_{AKmit}/FV_i \tag{27}$$

$$\frac{dPCr_i}{dt} = \frac{R_{PCr}}{L_i}(PCr - PCr_i) + v_{MiCK}/FV_i \tag{28}$$

$$\frac{dCr_i}{dt} = \frac{R_{Cr}}{L_i}(Cr - Cr_i) - v_{MiCK}/FV_i \tag{29}$$

$$\frac{dPi_i}{dt} = \frac{R_{Pi}}{L_i}(Pi - Pi_i) - v_{PI}/FV_i, \tag{30}$$

where v_{MiCK} is $MiCK$ reaction rate, v_{ANT} is the net rate of ATP export by ANT from matrix, v_{AKmit} is AK reaction rate (see eq. (14)), v_{PI} is the rate of the phosphate carrier in the inner membrane, L_i is the width of the layer between the inner and outer membranes, and FV_i is the fractional volume of the intermembrane space with respect to the cell volume.

The MiCK reaction rate v_{MiCK} is devided into v_{MiCKG} which involves micro-compartment ATP(ADP) and v_{MiCKI} which involves ATP(ADP) from the intermembrane space

$$v_{MiCK} = v_{MiCKG} + v_{MiCKI}. \tag{31}$$

The reaction rates are as follows

$$v_{MiCKG} = \left(V_1 \frac{mATP_g \cdot Cr_i}{K_{iaG} K_b} - V_{-1} \frac{mADP_g \cdot PCr_i}{K_{icG} K_d} \right) / DenMiCK, \tag{32}$$

$$v_{MiCKI} = \left(V_1 \frac{mATP_i \cdot Cr_i}{K_{ia} K_b} - V_{-1} \frac{mADP_i \cdot PCr_i}{K_{ic} K_d} \right) / DenMiCK, \tag{33}$$

where

$$\begin{aligned} DenMiCK \;=\; & \\ & 1 + Cr_i/K_{ib} + PCr_i/K_{id} + \\ & (mATP_g/K_{iaG} + mATP_i/K_{ia}) \cdot (1 + Cr_i/K_b) + \\ & (mADP_g/K_{icG} + mADP_i/K_{ic}) \cdot (1 + PCr_i/K_d + Cr_i/K_{Ib}). \end{aligned} \tag{34}$$

Restricted diffusion between the micro-compartment and the intermembrane space is governed by

$$v_{exchATP} = R_{exchATP} \cdot (ATP_i - ATP_g) \tag{35}$$

for ATP and

$$v_{exchADP} = R_{exchADP} \cdot (ADP_i - ADP_g) \tag{36}$$

for ADP.

For the oxydative phosphorylation, we use the model by Korzeniewski (22).

$$\frac{dUQ}{dt} = (v_{C3} - v_{C1})/FV_x \tag{37}$$

$$\frac{dc^{3+}}{dt} = 2(2v_{O_2} - v_{C3})/FV_x \tag{38}$$

$$\frac{dNAD^+}{dt} = (v_{C1} - v_{dh})/FV_x \tag{39}$$

$$\begin{aligned} \frac{dH_x}{dt} = & -(2(2+2u)v_{O_2} + 4v_{C1} + (4-2u)v_{C3} - n_a v_{sn} - \\ & v_{ANT}u - (1-u)v_{PI} - v_{leak})/(FV_x \cdot r_{buff}) \end{aligned} \tag{40}$$

$$\frac{dATP_x}{dt} = (v_{sn} - v_{ANT})/FV_x \tag{41}$$

$$\frac{dPi_x}{dt} = (v_{PI} - v_{sn})/FV_x. \tag{42}$$

Here are given the concentrations of the following metabolites: UQ — oxidized form of coenzyme Q; c^{3+} — oxidized form of cytochrome c; NAD^+ — NAD^+ in the matrix; H_x, ATP_x and Pi_x — H^+, ATP and Pi in the matrix, respectively. FV_x is the fractional volume of the mitochondrial matrix with respect to the cell volume. The following reaction rates are used in the above equations (22):

Substrate dehydrogenation

$$v_{dh} = \frac{k_{dh}}{\left(1 + \frac{K_{mN}}{NAD^+/NADH}\right)^{p_D}}. \tag{43}$$

Complex I

$$v_{C1} = k_{C1}(E_u - E_n - 2\Delta p). \tag{44}$$

Complex III

$$v_{C3} = k_{C3}(E_c - E_u - (2-u)\Delta p). \tag{45}$$

Complex IV

$$v_{O_2} = \frac{1}{2} k_{C4} \cdot a^{2+} \cdot c^{2+} \frac{O_2}{O_2 + k_{mO}}. \tag{46}$$

ATP synthase

$$v_{sn} = k_{sn} \frac{10^{\Delta G_{sn}/Z} - 1}{10^{\Delta G_{sn}/Z} + 1}. \tag{47}$$

Phosphate carrier

$$v_{PI} = v_{fPI} H_{ext} \frac{Pi_i}{1 + 10^{pH_{ext} - pK_a}} - v_{bPI} H_x \frac{Pi_x}{1 + 10^{pH_x - pK_a}}. \tag{48}$$

Proton leak

$$v_{leak} = k_{L1}(10^{k_{L2}\Delta p} - 1). \tag{49}$$

In eqs. (43)–(49), we used the total metabolite pools for substrate, coenzyme Q, cytochrome c, cytochrome a_3, and adenine nucleotides (in matrix) as follows.

$$\begin{aligned} NAD_{tot} &= NAD^+ + NADH, & (50)\\ UQ_{tot} &= UQ + UQH_2, & (51)\\ c_{tot} &= c^{3+} + c^{2+}, & (52)\\ a_{tot} &= (a^{3/2} + 1)\ a^{2+}, & (53)\\ A_x &= ATP_x + ADP_x. & (54) \end{aligned}$$

The concentrations of magnesium-bound and magnesium-free forms of adenine nucleotides in matrix are obtained using eqs. (10)–(13). For computing: pH in matrix pH_x, pH difference across the inner membrane ΔpH, protonmotive force Δp, electrical potential $\Delta\Psi$, and buffering rate r_{buff}, the following equations were used

$$\begin{aligned} pH_x &= -\log(H_x/\eta), & (55)\\ \Delta pH &= Z(pH_x - pH_{ext}), & (56)\\ \Delta p &= \frac{1}{1-u}\Delta pH, & (57)\\ \Delta\Psi &= -(\Delta p - \Delta pH), & (58)\\ H_{ext} &= \eta \cdot 10^{-pH_{ext}}, & (59)\\ r_{buff} &= r_{buff0} \cdot \eta \cdot \frac{dpH_x}{dH_x}. & (60) \end{aligned}$$

Here coefficient $u = \Delta\Psi/\Delta p$ is kept constant. Because of the high permeability of the mitochondrial outer membrane for protons, pH in intermembrane space pH_{ext} is considered being equal to that in cytoplasm and constant. The coefficient η is used to convert between molar concentrations and the concentrations used in the model (micromolars). The coefficient Z is expressed as

$$Z = \ln(10)\frac{RT}{F}, \tag{61}$$

where R is the gas constant, T is the absolute temperature and F is the Faraday's number. Throughout this text, the notations ln and log stand for logarithms on bases $e = 2.718\ldots$ and 10, respectively.

Description of ANT kinetics is based on the phenomenological model by Korzeniewski (22). The net rate of ATP export by ANT from matrix to micro-compartment and intermembrane space is

$$v_{ANT} = v_{ANT}^{X-G} + v_{ANT}^{X-I} \tag{62}$$

where v_{ANT}^{X-G} is the rate of ATP export by ANT from matrix to micro-compartment and v_{ANT}^{X-I} is the rate of ATP export by ANT from matrix directly to intermembrane space. These rates are described by the following kinetic equations

$$\begin{aligned} v_{ANT}^{X-G} &= V_{ANT} \cdot \frac{fADP_g}{K_g\,(1 + fADP_g/K_g + fADP_i/K_i)} \times \\ &\quad \times \left(\frac{fADP_g}{fATP_g 10^{+0.35\Delta\Psi/Z} + fADP_g} - \frac{fADP_x}{fATP_x 10^{-0.65\Delta\Psi/Z} + fADP_x} \right), \qquad (63) \\ v_{ANT}^{X-I} &= V_{ANT} \cdot \frac{fADP_i}{K_i\,(1 + fADP_g/K_g + fADP_i/K_i)} \times \\ &\quad \times \left(\frac{fADP_i}{fATP_i 10^{+0.35\Delta\Psi/Z} + fADP_i} - \frac{fADP_x}{fATP_x 10^{-0.65\Delta\Psi/Z} + fADP_x} \right). \qquad (64) \end{aligned}$$

The capacity of the micro-compartment is concidered to be infinitesimal. Therefore, for both ATP and ADP, the influx of the metabolite is balanced by its outflux,

$$\begin{aligned} -v_{MiCKG} + v_{ANT}^{X-G} + v_{exchATP} &= 0, \qquad (65) \\ v_{MiCKG} - v_{ANT}^{X-G} + v_{exchADP} &= 0. \qquad (66) \end{aligned}$$

The above equations can be solved for ATP_g and ADP_g using, for example, the Newton-Raphson method.

The thermodynamic span of ATP synthase is calculated as follows

$$\Delta G_{sn} = n_a \Delta p - \frac{\Delta G_0}{F} - Z \log \frac{\eta ATP_x}{ADP_x Pi_x}, \tag{67}$$

where n_a and ΔG_0 are the H^+/ATP stoichiometry and standard free energy for ATP synthase, respectively.

In eqs. (44) and (45) are used the NAD, coenzyme Q, and cytochrome c redox potentials

$$E_n = E_{n0} + \frac{Z}{2} \log \frac{NAD^+}{NADH}, \tag{68}$$

$$E_u = E_{u0} + \frac{Z}{2} \log \frac{UQ}{UQH_2}, \tag{69}$$

$$E_c = E_{c0} + Z \log \frac{c^{3+}}{c^{2+}}, \tag{70}$$

respectively. For computing the concentration of reduced cytochrome a_3 used in eq. (46), the redox potential of cytochrome a_3

$$E_a = E_c + (1 + u)\Delta p \tag{71}$$

is substituted into relation

$$a^{3/2} = 10^{(E_a - E_{a0})/Z}, \tag{72}$$

which gives the result (together with eq. (53)).

Assuming the infinitely fast diffusion, the 2D model can be simplified to the 0D model. In this model, the concentrations of the metabolites are spatially homogeneous and all the partial differential equations can be reduced to ordinary differential equations, hence the name. The 0D model is obtained by setting

$$\nabla^2 Met = 0 \tag{73}$$

in eqs. (1)–(6), integrating them over the region of myofibril and myoplasm and dividing by the area of this region. The integration of space-dependent functions G_{CK}, G_{AK} and G_H leads us to

$$F_{CK} = \frac{\iint G_{CK}(x,y)\,dx\,dy}{\iint dx\,dy} = 1, \tag{74}$$

$$F_{AK} = \frac{\iint G_{AK}(x,y)\,dx\,dy}{\iint dx\,dy} = 1 \tag{75}$$

and

$$F_H = \frac{\iint G_H(x,y)\,dx\,dy}{\iint dx\,dy} = \frac{1}{1.2}. \tag{76}$$

Zero-dimensional model

The concentrations of the free metabolites in cardiac myocytes are described by the following equations

$$\frac{dATP}{dt} = -F_{CK}v_{CK} + F_{AK}v_{AK} - F_H H_{ATP}(t) + \frac{R_{ATP}}{L_m}(ATP_i - ATP), \tag{77}$$

$$\frac{dADP}{dt} = F_{CK}v_{CK} - 2F_{AK}v_{AK} + F_H H_{ATP}(t) + \frac{R_{ADP}}{L_m}(ADP_i - ADP), \tag{78}$$

$$\frac{dAMP}{dt} = F_{AK}v_{AK} + \frac{R_{AMP}}{L_m}(AMP_i - AMP), \tag{79}$$

$$\frac{dPCr}{dt} = F_{CK}v_{CK} + \frac{R_{PCr}}{L_m}(PCr_i - PCr), \tag{80}$$

$$\frac{dCr}{dt} = -F_{CK}v_{CK} + \frac{R_{Cr}}{L_m}(Cr_i - Cr), \tag{81}$$

$$\frac{dPi}{dt} = F_H H_{ATP}(t) + \frac{R_{Pi}}{L_m}(Pi_i - Pi), \tag{82}$$

where L_m is the distance between the myofibrillar core and the mitochondrial membrane. In addition to eqs. (77)–(82) the complete 0D model includes eqs. (25)–(30) and (37)–(42).

Table 1

Event	Parameter	Dimension	Value
Diffusion			
	D_{ATP}	$\mu m^2/s$	$1.45 \cdot 10^2$
	D_{ADP}	$\mu m^2/s$	$1.45 \cdot 10^2$
	D_{AMP}	$\mu m^2/s$	$1.45 \cdot 10^2$
	D_{PCr}	$\mu m^2/s$	$2.6 \cdot 10^2$
	D_{Cr}	$\mu m^2/s$	$2.6 \cdot 10^2$
	D_{Pi}	$\mu m^2/s$	$3.27 \cdot 10^2$
CK in myofibril and myoplasm			
	V_1	$\mu M/s$	$1.30 \cdot 10^4$ *
		$mmol \cdot s^{-1} \cdot (kg\ wm)^{-1}$	6.0
	V_{-1}	$\mu M/s$	$5.48 \cdot 10^4$ *
		$mmol \cdot s^{-1} \cdot (kg\ wm)^{-1}$	25.2
	K_{ia}	μM	$9.0 \cdot 10^2$
	K_b	μM	$1.55 \cdot 10^4$
	K_{ic}	μM	$2.224 \cdot 10^2$
	K_d	μM	$1.67 \cdot 10^3$
	K_{ib}	μM	$3.49 \cdot 10^4$
	K_{id}	μM	$4.73 \cdot 10^3$
	K_{Ib}	μM	$3.49 \cdot 10^4$
CK in mitochondrion			
	V_1	$\mu M/s$	$7.07 \cdot 10^3$
		$mmol \cdot s^{-1} \cdot (kg\ wm)^{-1}$	4.0
	V_{-1}	$\mu M/s$	$2.97 \cdot 10^4$
		$mmol \cdot s^{-1} \cdot (kg\ wm)^{-1}$	16.8
	K_{ia}	μM	$7.12 \cdot 10^2$
	K_b	μM	$5.2 \cdot 10^3$
	K_{ic}	μM	$1.42 \cdot 10^2$
	K_d	μM	$5 \cdot 10^2$
	K_{ib}	μM	$2.6 \cdot 10^4$
	K_{id}	μM	$1.6 \cdot 10^3$
	K_{Ib}	μM	$2.6 \cdot 10^4$
	K_{iaG}	μM	$1.61 \cdot 10^2$
	K_{icG}	μM	$1.10 \cdot 10^4$
AK in myofibrils			
	k_{fa}	$1/(\mu M \cdot s)$	63.8
	k_{ba}	$1/(\mu M \cdot s)$	1.68
AK in mitochondrion			
	k_{fa}	$1/\mu M \cdot s)$	63.8
	k_{ba}	$1/\mu M \cdot s)$	1.68

Table 1 (continued)

Event	Parameter	Dimension	Value
Mg^{2+}, buffering			
	Mg_{ext}	μM	$1.0{\cdot}10^3$
	K_{DText}	μM	24.0
	K_{DDext}	μM	347.0
	Mg_x	μM	380.0
	k_{DTx}	μM	17.0
	k_{DDx}	μM	282.0
H^+, buffering			
	pH_{ext}		6.9
	r_{buff0}	M	0.022
ATP hydrolysis			
	$H_{ATP(max)}$	μM/s	$4.54{\cdot}10^4$
	$H_{ATP(base)}$	μM/s	153
Diffusion through mitochondrial outer membrane			
	L_i	μm	0.1
	L_m	μm	1.2
	R_{ATP}	μm/s	0.16
	R_{ADP}	μm/s	0.16
	R_{AMP}	μm/s	0.16
	R_{PCr}	μm/s	260
	R_{Cr}	μm/s	260
	R_{Pi}	μm/s	327
ATP diffusion between micro-compartment and intermembrane space			
	$R_{exchATP}$	1/s	1.88
	$R_{exchADP}$	1/s	1.88
ATP/ADP translocation by ANT			
	V_{ANT}	μM/s	$5.70{\cdot}10^3$
	K_g	μM	4.25
	K_i	μM	4.25

Table 1 (continued)

Event	Parameter	Dimension	Value
Respiratory chain			
	k_{dh}	μM/s	$5.75{\cdot}10^4$
	K_{mN}		100.0
	p_D		0.8
	k_{C1}	μM/s	$2.0{\cdot}10^2$
	k_{C3}	μM/s	$1.142{\cdot}10^2$
	k_{C4}	$1/(\mu\text{M}\cdot\text{ s})$	2.351
	k_{mO}	μM	150.0
	E_{n0}	mV	-320.0
	E_{u0}	mV	85.0
	E_{c0}	mV	250.0
	E_{a0}	mV	540.0
	NAD_{tot}	μM	$2.97{\cdot}10^3$
	UQ_{tot}	μM	$1.35{\cdot}10^3$
	c_{tot}	μM	$2.7{\cdot}10^2$
	a_{tot}	μM	$1.35{\cdot}10^2$
	O_2	μM	$2.4{\cdot}10^2$
ATP synthesis			
	k_{sn}	μM/s	$2.96{\cdot}10^4$
	ΔG_0	kJ/mol	31.9
	n_a		2.5
	A_x	μM	$1.0{\cdot}10^4$
Phosphate carrier			
	v_{fPI}	$1/(\mu\text{M}\cdot\text{ s})$	138.5
	v_{bPI}	$1/(\mu\text{M}\cdot\text{ s})$	138.5
	pK_a		6.8
Proton leak			
	k_{L1}	μM/s	$2.1895{\cdot}10^3$
	k_{L2}	1/mV	0.003
General constants			
	T	K	298
	R	kJ/(mol$\cdot$ K)	0.0083
	F	kJ/(mol$\cdot$ mV)	0.0965
	Z	mV	$\ln(10)RT/F$
	u		0.861
	η		10^6
Fractional volumes			
	FV_x		3/16
	FV_i		1/16

Table 1 (continued)

* CK reaction rates are given in units of μM/s for concentration change in myofibrillar and cytoplasmic compartment.