A Matlab program for calculation the interrelationship of the rate of ATP synthesis (oxygen consumption) based on the cytochrome c oxidase model of Wilson and Vinogradov (2-4) as adapted for cellular energy metabolism (1, 5).

\[
\begin{align*}
K_e &= 6.4 \times 10^{11}; \\
k_1 &= 8 \times 10^9; \\
k_{1r} &= 8 \times 10^7; \\
k_2 &= 6 \times 10^8; \\
k_{2r} &= 1 \times 10^1; \\
K_3 &= 1 \times 10^6; \\
K_5 &= 1 \times 10^25; \\
k_{4a} &= 2 \times 10^7; \\
k_{4b} &= 3 \times 10^8; \\
a_{3t} &= 1 \times 10^{-6}; \text{ % total cyt a}_3 \text{ concentration} \\
c_t &= 2 \times 10^{-6}; \text{ % total cyt. c concentration (2 x total cyt a}_3) \\
NADt &= 2 \times 10^{-5}; \text{ % total nad pool ([NAD+] + [NADH])} \\
x &= (1:50)'; \text{ % used to generate levels for [CrP] (as well as [Cr] and [Pi])} \\
\text{for } q = 1:4; \text{ % used to generate levels of reactant 2-undefined in this case} \\
W &= 7.1; \text{ % W = intracellular pH} \\
H &= 10^{-W}; \text{ % H = hydrogen ion concentration} \\
NADH &= 0.5 \times 10^{-6}; \text{ % sets intramitochondrial NADH} \\
NAD &= NADt - NADH; \text{ % calculated intramitochondrial NAD}^+ \\
CrP &= 34.4 - x \times 0.4; \text{ % calculates [CrP]} \\
Cr &= 11.6 + x \times 0.4; \text{ % calculated [Cr]} \\
Pi &= 2.6 + x \times 0.4; \text{ % calculates [Pi]} \\
M &= (CrP/(Cr .* Pi)).10^3; \text{ % creatine energy state in mM} \\
J &= M \times 142; \text{ % ATP energy state in Molar} \\
L &= 1.42 \times \log10(J); \% \\
N &= 7.5 + L; \text{ % calculates free energy} \\
Q &= N ./ 46.183; \text{ % energy state in volts} \\
O &= 35.10^{-6}; \text{ % O is the oxygen concentration} \\
G &= Q * 46.183; \text{ % Gibb's free energy in kcal} \\
S &= Q ./ 0.059; \text{ % for energy conservation} \\
z &= 10^{-S}; \text{ % for energy coupling} \\
kf_1 &= k_1 ./ z \times 0.5; \% \text{ couples k1 to energy state} \\
k_{1r} &= k_{1r} \times z \times 0.5; \% \text{ couples k1r to energy state} \\
D &= (NAD/NADH)^{0.5} \times z \times 2 \times (H./K_e)^{0.5}; \\
c_o &= D \times ct/(1 + D); \% \text{ co is the concentration of oxidized cyt c} \\
cr &= ct - co; \% \text{ cr is the concentration of reduced cyt c} \\
A &= (k2r + k4a \times cr + k4b \times cr \times K3 \times H)/(k2 \times O); \% \text{ variable A in SS exp} \\
B &= (k2 \times O \times A + k1 \times co \times A - k2r)/(kf1 \times cr); \% \text{ var. B in SS rate exp} \\
C &= K5 \times 1 \times (1/H)^{2} \times co/ct \times z \times 2 \times B; \% \text{ var. C in SS rate exp} \\
III &= a_{3t} / (1 + K3 \times H + A + B + C); \% \text{ calc conc. of intermediate III} \\
I &= B \times III; \% \text{ calc. conc. of intermediate I} \\
II &= A \times III; \% \text{ calc. conc. of intermediate II} \\
IV &= K3 \times H \times III; \% \text{ calc. conc. of intermediate IV} \\
V &= C \times III; \% \text{ calc. conc. of intermediate V} \\
y(q,x) &= (k4a \times cr + k4b \times cr \times K3 \times H) \times III \times 4/ct; \% \text{ rate cyt c TN exp} \\
\end{align*}
\]

end

plot (x,y) \% plots cyt c TN vs x value
axis([0 50 0 35]) \% sets graph x and y axis limits

The program is written to calculate a number of different metabolic parameters as well as the intermediates in the cytochrome c oxidase reaction. As shown, the variable q is not defined so 4 identical calculations will be made. A range of values for q can be entered and used to determine the dependence on any other variable,
such as energy state, oxygen concentration, etc. Note that the pH dependence includes only that for the cytochrome c oxidase reaction. The pH dependencies due to ATP hydrolysis etc are not included. The equilibrium constant $K_e$ for the first two sites of oxidative phosphorylation is for pH 7.1. If the intramitochondrial pH (7.5?) is used the equilibrium constant for pH 7.5 should be used and the $[\text{NAD}^+]/[\text{NADH}]$ adjusted to provide the same redox potential for the intramitochondrial NAD couple as for the indicated $K_e$ and $[\text{NAD}^+]/[\text{NADH}]$ for pH 7.1.


