

Supplementary Table 4:

Equations governing the dynamics of the carbohydrate metabolism:

$$\frac{d}{dt}Gluc = v_1 - v_2 - Gluc \cdot V_{ratio} \quad (5.1)$$

$$\frac{d}{dt}G6P = v_2 - v_3 - v_{10} - G6P \cdot V_{ratio} \quad (5.2)$$

$$\frac{d}{dt}FBP = v_3 - v_4 - FBP \cdot V_{ratio} \quad (5.3)$$

$$\frac{d}{dt}GAP = v_4 + v_5 - v_6 - GAP \cdot V_{ratio} \quad (5.4)$$

$$\frac{d}{dt}DHAP = v_4 - v_5 - v_{11} - DHAP \cdot V_{ratio} \quad (5.5)$$

$$\frac{d}{dt}Pyr = v_6 - v_7 - v_8 - v_9 - Pyr \cdot V_{ratio} \quad (5.6)$$

$$\frac{d}{dt}G3P = v_{11} - v_{12} - G3P \cdot V_{ratio} \quad (5.7)$$

$$\frac{d}{dt}Glyc = v_{12} - v_{13} - Glyc \cdot V_{ratio} \quad (5.8)$$

$$\frac{d}{dt}Glyc_{ex} = \frac{v_{13}}{k_x} \quad (5.9)$$

$$\frac{d}{dt}NADH = v_6 + 4 \cdot v_7 - v_8 - v_{11} - v_{14} + v_{15} - NADH \cdot V_{ratio} \quad (5.10)$$

$$\frac{d}{dt}NAD^+ = -v_6 - 4 \cdot v_7 + v_8 + v_{11} + v_{14} - v_{15} - NAD^+ \cdot V_{ratio} \quad (5.11)$$

$$\frac{d}{dt}ATP = -v_2 - v_3 + 2 \cdot v_6 + v_7 - v_9 - v_{10} + 3 \cdot v_{14} - v_{16} - ATP \cdot V_{ratio} \quad (5.12)$$

$$\frac{d}{dt}ADP = v_2 + v_3 - 2 \cdot v_6 - v_7 + v_9 + v_{10} - 3 \cdot v_{14} + v_{16} - ADP \cdot V_{ratio} \quad (5.13)$$

$$v_1 = \frac{Protein_1}{Protein_1^0} \cdot v_1^0 \quad (5.14)$$

$$v_2 = \frac{Protein_1}{Protein_1^0} \frac{k_2}{\left(1 + \frac{k_{21}}{ATP} \left(1 + \frac{ADP}{k_{22}}\right) + \frac{k_{23}}{Gluc} + \frac{k_{21}}{ATP} \cdot \frac{k_{23}}{Gluc} \cdot \left(1 + \frac{ADP}{k_{22}}\right)\right)} \quad (5.15)$$

$$v_3 = k_3 \cdot \frac{ATP}{(k_{31} + ATP)} \cdot \frac{G6P}{(k_{32} + G6P)} \quad (5.16)$$

$$v_4 = k_4 \cdot \frac{\left(FBP - \frac{GAP \cdot DHAP}{K_{eq,4}}\right)}{\left(k_{FBP,4} + FBP + \frac{k_{DHAP,4} \cdot GAP}{K_{eq,4} \cdot v_{bf,4}} + \frac{k_{GAP,4}}{K_{eq,4} \cdot v_{bf,4}} + \frac{FBP \cdot GAP}{K_{IGAP,4}} + \frac{GAP \cdot DHAP}{K_{eq,4} \cdot v_{bf,4}}\right)} \quad (5.17)$$

$$v_5 = k_5 \cdot \frac{DHAP - \frac{GAP}{K_{eq,5}}}{\left(K_{DHAP,5} \cdot \left(1 + \frac{GAP}{K_{GAP,5}}\right) + DHAP\right)} \quad (5.18)$$

$$v_6 = k_6 \cdot GAP \cdot NAD \cdot ADP \quad (5.19)$$

$$v_7 = k_7 \cdot \frac{ADP \cdot Pyr \cdot NAD}{\left(K_{NAD,7} \cdot Pyr + K_{Pyr,7} \cdot NAD + K_{I,7} \cdot NADH\right)} \quad (5.20)$$

$$v_8 = k_8 \cdot \frac{Pyr}{(k_{81} + Pyr)} \cdot \frac{NAD}{(k_{82} + NAD)} \quad (5.21)$$

$$v_9 = k_9 \cdot \frac{Pyr}{(K_{Pyr,9} + Pyr)} \cdot \frac{ATP}{(K_{ATP,9} + ATP)} \quad (5.22)$$

$$v_{10} = k_{10} \cdot \frac{G6P}{(K_{G6P,10} + G6P)} \cdot \frac{ATP}{(K_{ATP,10} + ATP)} \quad (5.23)$$

$$v_{11} = \frac{Protein_1}{Protein_1^0} \cdot k_{11} \cdot \frac{DHAP \cdot NADH - \frac{G3P \cdot NAD}{K_{eq,11}}}{\left(1 + \frac{DHAP}{k_{d,11}} + \frac{NADH}{k_{n,11}} + \frac{G3P \cdot NAD}{k_{h,11}}\right)} \quad (5.24)$$

$$v_{12} = \frac{Protein_1}{Protein_1^0} \cdot k_{12} \cdot G3P \quad (5.25)$$

$$v_{13} = k_{13}(t) \cdot (Glyc - Glyc_{ex}) \quad (5.26)$$

$$\text{with } k_{13}(t) = k_{13}^0 \cdot \left(\frac{\Pi_t(t)}{\Pi_t^0} \right)^{n_{13}} \quad (\text{compare with main text})$$

$$v_{14} = k_{14} \cdot \frac{NADH \cdot ADP}{(K_{ADP,14} + ADP)} \quad (5.27)$$

$$v_{15} = k_{15} \cdot NAD \quad (5.28)$$

$$v_{16} = k_{16} \cdot \frac{ATP}{(K_{ATP,16} + ATP)} \quad (5.29)$$

Parameters

$$v_1^0 = 1.296 \text{mM} \cdot \text{s}^{-1}$$

$$k_2 = 1.777 \text{mM} \cdot \text{s}^{-1}$$

$$k_{21} = 0.2 \text{mM}$$

$$k_{22} = 1.2 \text{mM}$$

$$k_{23} = 0.2 \text{mM}$$

$$k_3 = 0.895 \text{mM} \cdot \text{s}^{-1}$$

$$k_{31} = 0.01 \text{mM}$$

$$k_{32} = 0.012 \text{mM}$$

$$k_4 = 1.8764 \cdot 10^3 \text{mM} \cdot \text{s}^{-1}$$

$$K_{eq,4} = 0.81 \text{mM}$$

$$k_{FBP,4} = 0.054 \text{mM}$$

$$k_{DHAP,4} = 2.0 \text{mM}$$

$$k_{GAP,4} = 2.0 \text{mM}$$

$$v_{bf,4} = 5.0 \text{mM}^{-1}$$

$$K_{IGAP,4} = 10.0 \text{mM}$$

$$k_5 = 190 \text{mM} \cdot \text{s}^{-1}$$

$$K_{eq,5} = 0.045$$

$$K_{DHAP,5} = 0.38 \text{mM}$$

$$K_{GAP,5} = 0.064 \text{mM}$$

$$k_6 = 45.127 \text{mM}^{-2} \text{s}^{-1}$$

$$k_7 = 639.137 \text{s}^{-1}$$

$$K_{Pyr,7} = 70.0 \text{mM}$$

$$K_{NAD,7} = 160.0 \text{mM}$$

$$K_{I,7} = 20.0 \text{mM}$$

$$k_8 = 5.6425 \text{mM} \cdot \text{s}^{-1}$$

$$k_{81} = 1.2 \text{mM}$$

$$k_{82} = 0.6 \text{mM}$$

$$k_9 = 0.8090 \text{mM} \cdot \text{s}^{-1}$$

$$K_{Pyr,9} = 0.92 \text{mM}$$

$$K_{ATP,9} = 13.2 \text{mM}$$

$$k_{10} = 1.9377 \text{mM} \cdot \text{s}^{-1}$$

$$K_{G6P,10} = 2.7 \text{mM}$$

$$K_{ATP,10} = 0.4 \text{mM}$$

$$k_{11} = 7.1507 (\text{mM} \cdot \text{s})^{-1}$$

$$k_{d,11} = 0.0037 \text{mM}$$

$$k_{n,11} = 0.6 \text{mM}$$

$$k_{h,11} = 0.2 \text{mM}$$

$$K_{eq,11} = 37$$

$$k_{12} = 0.0162 \text{s}^{-1}$$

$$k_{13}^0 = 0.005 \text{s}^{-1}$$

$$k_x = 6.67 \cdot 10^{-10}$$

$$n_{13} = 4$$

$$k_{14} = 384.024 \text{s}^{-1}$$

$$K_{ADP,14} = 0.42 \text{mM}$$

$$k_{15} = 1.1235 \text{s}^{-1}$$

$$k_{16} = 99.887 \text{mM} \cdot \text{s}^{-1}$$

$$K_{ATP,16} = 5.0 \text{mM}$$

Initial concentration values

$$Gluc^0 = 1mM$$

$$G6P^0 = 0.93mM$$

$$FBP^0 = 0.11mM$$

$$GAP^0 = 0.063mM$$

$$DHAP^0 = 1.41mM$$

$$Pyr^0 = 0.79mM$$

$$G3P^0 = 0.063mM$$

$$Glyc_{in}^0 = 0.2mM$$

$$Glyc_{ex}^0 = 0.2mM$$

$$NADH^0 = 0.04mM$$

$$NAD^0 = 1.03mM$$

$$ATP^0 = 2.1mM$$

$$ADP^0 = 0.6mM$$