

# beard\_model\_2005

## 1 “Environment” component

This component has no equations.

## 2 “Fixed\_parameters” component

H\_e\_Eqn

$$H_e = (10)^{-(pH_e)}$$

W\_x\_Eqn

$$W_x = 0.9 * W_m$$

W\_i\_Eqn

$$W_i = 0.1 * W_m$$

H\_i\_Eqn

$$H_i = H_e$$

K\_i\_Eqn

$$K_i = K_e$$

## 3 “Adjustable\_parameters” component

This component has no equations.

## 4 “Dehydrogenase\_flux” component

J\_DH\_Eqn

$$J_{DH} = x_{DH} * (r * NAD_x - NADH_x) * \frac{\left(1 + \frac{P_{i,x}}{k_{Pi1}}\right)}{\left(1 + \frac{P_{i,x}}{k_{Pi2}}\right)}$$

## 5 “dH\_x\_dt” component

H\_x\_diff\_eqn

$$\frac{d(H_x)}{d(t)} = x_{buf} f_{H_x} * \frac{(((((((J_{DH} - 5 * J_{C1}) - 2 * J_{C3}) - 4 * J_{C4}) + (n_A - 1) * J_{F1}) + 2 * J_{Pi1}) + J_{Hle}) - J_{KH})}{W_x}$$

## 6 “dK\_x\_dt” component

K\_x\_diff\_Eqn

$$\frac{d(K_x)}{d(t)} = \frac{(J_{KH} + J_K)}{W_x}$$

## 7 “dMg\_x\_dt” component

Mg\_x\_diff\_Eqn

$$\frac{d(Mg_x)}{d(t)} = \frac{-(J_{MgATPx}) - J_{MgADPx}}{W_x}$$

## 8 “dNADH\_x\_dt” component

NADH\_x\_diff\_Eqn

$$\frac{d(NADH_x)}{d(t)} = \frac{(J_{DH} - J_{C1})}{W_x}$$

## 9 “dQH2\_dt” component

QH2\_diff\_Eqn

$$\frac{d(QH2)}{d(t)} = \frac{(J_{C1} - J_{C3})}{W_x}$$

## 10 “dCred\_dt” component

Cred\_diff\_Eqn

$$\frac{d(Cred)}{d(t)} = \frac{(2 * J_{C3} - 2 * J_{C4})}{W_i}$$

## 11 “dATP\_x\_dt” component

ATP\_x\_diff\_Eqn

$$\frac{d(ATP_x)}{d(t)} = \frac{(J_{F1} - J_{ANT})}{W_x}$$

## 12 “dADP\_x\_dt” component

ADP\_x\_diff\_Eqn

$$\frac{d(ADP_x)}{d(t)} = \frac{-(J_{F1}) + J_{ANT}}{W_x}$$

## 13 “dATP\_mx\_dt” component

ATP\_mx\_diff\_Eqn

$$\frac{d(ATP_{mx})}{d(t)} = \frac{J_{MgATPx}}{W_x}$$

## 14 “dADP\_mx\_dt” component

ADP\_mx\_diff\_Eqn

$$\frac{d(ADP_{mx})}{d(t)} = \frac{J_{MgADPx}}{W_x}$$

## 15 “dPi\_x\_dt” component

Pi\_x\_diff\_Eqn

$$\frac{d(Pi_x)}{d(t)} = \frac{-(J_{F1}) + J_{Pi1}}{W_x}$$

## 16 “dATP\_i\_dt” component

ATP\_i\_diff\_Eqn

$$\frac{d(ATP_i)}{d(t)} = \frac{((J_{ATP} + J_{ANT}) + J_{AKi})}{W_i}$$

## 17 “dADP\_i\_dt” component

ADP\_i\_diff\_Eqn

$$\frac{d(ADP_i)}{d(t)} = \frac{((J_{ADP} - J_{ANT}) - 2 * J_{AKi})}{W_i}$$

## 18 “dAMP\_i\_dt” component

AMP\_i\_diff\_Eqn

$$\frac{d(AMP_i)}{d(t)} = \frac{(J_{AMP} + J_{AKi})}{W_i}$$

## 19 “dATP\_mi\_dt” component

ATP\_mi\_diff\_Eqn

$$\frac{d(ATP_mi)}{d(t)} = \frac{J_{MgATPi}}{W_i}$$

## 20 “dADP\_mi\_dt” component

ADP\_mi\_diff\_Eqn

$$\frac{d(ADP_mi)}{d(t)} = \frac{J_{MgADPi}}{W_i}$$

## 21 “dPi\_i\_dt” component

Pi\_i\_diff\_Eqn

$$\frac{d(Pi_i)}{d(t)} = \frac{(-(J_{Pi1}) + J_{Pi2})}{W_i}$$

## 22 “dPsi\_dt” component

dPsi\_diff\_Eqn

$$\frac{d(dPsi)}{d(t)} = 1.48e5 * (((((4 * J_{C1} + 2 * J_{C3}) + 4 * J_{C4}) - n_A * J_{F1}) - J_{ANT}) - J_{Hle}) - J_{K})$$

## 23 “dO2\_dt” component

O2\_diff\_Eqn

$$\frac{d(O_2)}{d(t)} = 0$$

## 24 “Electron\_flux\_complex\_I” component

dG\_C1op\_Eqn

$$dG_{C1op} = \left( \left( dG_{C1o} - 1 * RT * \ln \frac{H_x}{1e-7} \right) - RT * \ln \frac{Q}{QH2} \right)$$

J\_C1\_Eqn

$$J_{C1} = x_{C1} * \left( e^{-\left( \frac{dG_{C1op} + 4 * dG_{H}}{RT} \right)} * NADH_x - NAD_x \right)$$

## 25 “Proton\_motive\_energy” component

dG\_H\_Eqn

$$dG_H = \left( F * dPsi + RT * \ln \frac{H_i}{H_x} \right)$$

## 26 “Electron\_flux\_complex\_III” component

dG\_C3op\_Eqn

$$dG_{C3op} = \left( \left( dG_{C3o} + 2 * RT * \ln \frac{H_x}{1e-7} \right) - RT * \ln \frac{QH2}{Q} \right)$$

J\_C3\_Eqn

$$J_{C3} = x_{C3} * \frac{\left( 1 + \frac{Pi_x}{k_{Pi3}} \right)}{\left( 1 + \frac{Pi_x}{k_{Pi4}} \right)} * \left( e^{-\left( \frac{dG_{C3op} + 4 * dG_H - 2 * F * dPsi}{2 * RT} \right)} * Cox - Cred \right)$$

## 27 “Electron\_flux\_complex\_IV” component

dG\_C4op\_Eqn

$$dG_{C4op} = \left( \left( dG_{C4o} - 2 * RT * \ln \frac{H_x}{1e-7} \right) - \frac{RT}{2} * \ln O_2 \right)$$

**J\_C4\_Eqn**

$$J_{C4} = x_{C4} * \frac{1}{(1 + \frac{k_{O2}}{O2})} * \frac{C_{red}}{C_{tot}} * \left( e^{-\left(\frac{dG_{C4op} + 2 * dG_{-H}}{2 * RT}\right)} * C_{red} - C_{ox} * e^{F * \frac{dP_{Si}}{RT}} \right)$$

## 28 “ATP\_synthesis\_flux” component

**J\_F1\_Eqn**

$$J_{F1} = x_{F1} * \left( e^{-\left(\frac{dG_{F1o-n-A} * dG_{-H}}{RT}\right)} * \frac{K_{DD}}{K_{DT}} * ADP_{mx} * Pi_x - ATP_{mx} \right)$$

## 29 “MgATPx\_binding\_flux” component

**ATP\_fx\_Eqn**

$$ATP_{fx} = (ATP_x - ATP_{mx})$$

**J\_MgATPx\_Eqn**

$$J_{MgATPx} = x_{MgA} * (ATP_{fx} * Mg_x - K_{DT} * ATP_{mx})$$

## 30 “MgADPx\_binding\_flux” component

**ADP\_fx\_Eqn**

$$ADP_{fx} = (ADP_x - ADP_{mx})$$

**J\_MgADPx\_Eqn**

$$J_{MgADPx} = x_{MgA} * (ADP_{fx} * Mg_x - K_{DD} * ADP_{mx})$$

## 31 “MgATPi\_binding\_flux” component

**ATP\_fi\_Eqn**

$$ATP_{fi} = (ATP_i - ATP_{mi})$$

**J\_MgATPi\_Eqn**

$$J_{MgATPi} = x_{MgA} * (ATP_{fi} * Mg_i - K_{DT} * ATP_{mi})$$

### 32 “MgADPi\_binding\_flux” component

ADP.fi.Eqn

$$ADP\_fi = (ADP\_i - ADP\_mi)$$

J.MgADPi.Eqn

$$J\_MgADPi = x\_MgA * (ADP\_fi * Mg\_i - K\_DD * ADP\_mi)$$

### 33 “ATP\_substrate\_flux” component

J.ATP.Eqn

$$J\_ATP = gamma * x\_A * (ATP\_e - ATP\_i)$$

### 34 “ADP\_substrate\_flux” component

J.ADP.Eqn

$$J\_ADP = gamma * x\_A * (ADP\_e - ADP\_i)$$

### 35 “AMP\_substrate\_flux” component

J.AMP.Eqn

$$J\_AMP = gamma * x\_A * (AMP\_e - AMP\_i)$$

### 36 “Pi\_substrate\_flux” component

J.Pi2.Eqn

$$J\_Pi2 = gamma * x\_Pi2 * (Pi\_e - Pi\_i)$$

### 37 “ANT\_flux” component

Psi.x.Eqn

$$Psi\_x = -(0.65) * dPsi$$

Psi.i.Eqn

$$Psi\_i = 0.35 * dPsi$$

**J\_ANT\_Eqn**

$$J_{ANT} = \begin{cases} x_{ANT} * \left( \frac{ADP_{fi}}{(ADP_{fi} + ATP_{fi} * e^{-(F) * \frac{P_{si_i}}{RT}})} - \frac{ADP_{fx}}{(ADP_{fx} + ATP_{fx} * e^{-(F) * \frac{P_{si_x}}{RT}})} \right) * \frac{ADP_{fi}}{(ADP_{fi} + k_m ADP)}; & \text{if } (ADP_{fi} > 1E - 12) \vee (ATP_{fi} > 1E - 12), \\ 0 & \text{otherwise.} \end{cases}$$

### 38 “Phosphate\_hydrogen\_cotransporter\_flux” component

**H2PIi\_Eqn**

$$H2PIi = Pi_i * \frac{H_i}{(H_i + k_d HPI)}$$

**H2PIx\_Eqn**

$$H2PIx = Pi_x * \frac{H_x}{(H_x + k_d HPI)}$$

**J\_Pi1\_Eqn**

$$J_{Pi1} = x_{Pi1} * \frac{(H_x * H2PIi - H_i * H2PIx)}{(H2PIi + k_{PiH})}$$

### 39 “Adenylate\_kinase\_flux” component

**J\_AKi\_Eqn**

$$J_{AKi} = x_{AK} * (K_{AK} * ADP_i * ADP_i - AMP_i * ATP_i)$$

### 40 “Hydrogen\_leak\_flux” component

**J\_Hle\_Eqn**

$$J_{Hle} = x_{Hle} * dPsi * \frac{(H_i * e^{F * \frac{dPsi}{RT}} - H_x)}{(e^{F * \frac{dPsi}{RT}} - 1)}$$

### 41 “Passive\_potassium\_flux” component

**J\_K\_Eqn**

$$J_K = x_K * dPsi * \frac{(K_i * e^{F * \frac{dPsi}{RT}} - K_x)}{(e^{F * \frac{dPsi}{RT}} - 1)}$$

## 42 “Potassium\_hydrogen\_flux” component

J\_KH\_Eqn

$$J_{KH} = x_{KH} * (K_i * H_x - K_x * H_i)$$

## 43 “NAD\_x\_concentration” component

NAD\_x\_Eqn

$$NAD_x = (NAD_{tot} - NADH_x)$$

## 44 “Q\_concentration” component

Q\_Eqn

$$Q = (Q_{tot} - QH_2)$$

## 45 “Cox\_concentration” component

Cox\_Eqn

$$Cox = (C_{tot} - C_{red})$$

## 46 “ADP\_binding” component

ADP\_fe\_Eqn

$$ADP_{fe} = (ADP_e - ADP_{me})$$

ADP\_me\_Eqn

$$ADP_{me} = \frac{\left( \left( (K_{DD} + ADP_e) + Mg_{tot} \right) - \left( \left( \left( (K_{DD} + ADP_e) + Mg_{tot} \right)^2 - 4 * Mg_{tot} * ADP_e \right) \right)^{0.5} \right)}{2}$$

## 47 “Mg\_binding” component

Mg\_e\_Eqn

$$Mg_e = (Mg_{tot} - ADP_{me})$$

Mg\_i\_Eqn

$$Mg_i = Mg_e$$