

1 “global_variables” component

This component has no equations.

2 “volumes” component

This component has no equations.

3 “Glc_o” component

This component has no equations.

4 “Glc_i” component

$$\frac{d(\text{Glc}_i)}{d(\text{time})} = (V_{\text{glucose_transport}} - V_{\text{HK}})$$

5 “Glc_6_P_g” component

$$\text{Glc}_6\text{P}_g = \frac{\text{hexose}_P_g}{K_{eq_PGI}}$$

$$K_{eq_PGI} = \frac{\text{Fru}_6\text{P}_g}{\text{Glc}_6\text{P}_g}$$

6 “Fru_6_P_g” component

$$Fru_6_P_g = \frac{hexose_P_g}{Glc_6_P_g}$$

7 “hexose_P_g” component

$$\frac{d(hexose_P_g)}{d(time)} = (V_{HK} - V_{PFK})$$

8 “Fru_1_6_BP_g” component

$$\frac{d(Fru_1_6_BP_g)}{d(time)} = (V_{PFK} - V_{ALD})$$

9 “GA_3_P_g” component

$$GA_3_P_g = K_{eq_TIM} * DHAP_g$$

10 “triose_P” component

$$\frac{d(triose_P)}{d(time)} = ((2.0 * V_{ALD} + V_{GPO}) - (V_{GAPDH} + V_{GDH}))$$

11 “one_three_BPGA_g” component

$$\frac{d(one_three_BPGA_g)}{d(time)} = (V_{GAPDH} - V_{PGK})$$

12 “three_PGA” component

$$three_PGA = \frac{N * \left(1.0 + \frac{V_c}{V_g}\right)}{\left(1.0 + \left(1.0 + K_{eq_PGM} + K_{eq_PGM} * K_{eq_ENO}\right) * \frac{V_c}{V_g}\right)}$$

13 “two_PGA_c” component

$$two_PGA_c = Keq_PGM * three_PGA$$

14 “N” component

$$\frac{d(N)}{d(time)} = (V_PGK - V_PYK)$$

15 “PEP_c” component

$$PEP_c = Keq_ENO * two_PGA_c$$

16 “PYR_c” component

$$\frac{d(PYR_c)}{d(time)} = (V_PYK - V_pyruvate_transport)$$

17 “pyruvate_o” component

This component has no equations.

18 “glycerol_g” component

This component has no equations.

19 “DHAP_c” component

$$DHAP_c = \frac{\left(-\left(\left(\left(Q * \left(1.0 + Keq_TIM \right) + \frac{Vc}{Vg} * C5 \right) - triose_P * \left(1.0 + \frac{Vc}{Vg} \right) * Keq_TIM \right) \right) + \left(\left(\left(\left(\left(Q * \left(1.0 + Keq_TIM \right) + \frac{Vc}{Vg} * C5 \right) - triose_P * \left(1.0 + \frac{Vc}{Vg} \right) * Keq_TIM \right) \right) \right) \right)}{2.0 * Keq_TIM * \frac{Vc}{Vg}}$$

20 “DHAP_g” component

$$DHAP_g = \frac{Q * DHAP_c}{(C5 + Keq_TIM * DHAP_c)}$$

21 “Q” component

$$Q = (DHAP_g + GA3_P_g + Gly3_P_g)$$

22 “Gly_3_P_c” component

$$Gly3_P_c = (C5 - DHAP_c)$$

23 “Gly_3_P_g” component

$$Gly3_P_g = (Q - (DHAP_g + GA3_P_g))$$

24 “H2O” component

This component has no equations.

25 “O2” component

This component has no equations.

26 “NAD_g” component

$$NAD_g = (C3 - NADH_g)$$

27 “NADH_g” component

$$\frac{d(NADH_g)}{d(time)} = (V_{GAPDH} - V_{GDH})$$

28 “P_g” component

$$\frac{d(P_g)}{d(time)} = ((V_{PGK} + V_{GK}) - (V_{HK} + V_{PFK}))$$

29 “P_c” component

$$\frac{d(P_c)}{d(time)} = (V_{PYK} - V_{ATP_utilisation})$$

30 “ATP_g” component

$$ATP_g = \frac{\left((C1 - -(P_g * (1.0 - 4.0 * Keq_{AK}))) + \left(\left((C1 - -(P_g * (1.0 - 4.0 * Keq_{AK})))^{2.0} - 4.0 * (1.0 - 4.0 * Keq_{AK}) * -(Keq_{AK}) * (P_g)^{2.0} \right)^{0.5} \right) \right)}{2.0 * (1.0 - 4.0 * Keq_{AK})}$$

31 “ATP_c” component

$$ATP_c = \frac{\left((C1 - -(P_c * (1.0 - 4.0 * Keq_{AK}))) + \left(\left((C1 - -(P_c * (1.0 - 4.0 * Keq_{AK})))^{2.0} - 4.0 * (1.0 - 4.0 * Keq_{AK}) * -(Keq_{AK}) * (P_c)^{2.0} \right)^{0.5} \right) \right)}{2.0 * (1.0 - 4.0 * Keq_{AK})}$$

32 “ADP_g” component

$$ADP_g = (P_g - 2.0 * ATP_g)$$

33 “ADP_c” component

$$ADP_c = (P_c - 2.0 * ATP_c)$$

34 “AMP_g” component

$$AMP_g = (C1 - (ATP_g + ADP_g))$$

35 “AMP_c” component

$$AMP_c = (C2 - (ATP_c + ADP_c))$$

36 “C1” component

$$C1 = (ATP_g + ADP_g + AMP_g)$$

37 “C2” component

$$C2 = (ATP_c + ADP_c + AMP_c)$$

38 “C3” component

$$C3 = (NADH_g + NAD_g)$$

39 “C4” component

$$C4 = (Gly_3_P_g + DHAP_g + Glc_6_P_g + Fru_6_P_g + 2.0 * Fru_1_6_BP_g + GA_3_P_g + one_three_BPGA_g + 2.0 * ATP_g + ADP_g)$$

40 “C5” component

$$C5 = (Gly_3_P_c + DHAP_c)$$

41 “V_glucose_transport” component

V_glucose_transport_calculation

$$V_glucose_transport = V_glucose_transport_max * \frac{(Glc_o - Glc_i)}{\left(K_Glc + Glc_o + Glc_i + \alpha * Glc_o * \frac{Glc_i}{K_Glc}\right)}$$

42 “V_pyruvate_transport” component

V_pyruvate_transport_calculation

$$V_pyruvate_transport = V_pyruvate_transport_max * \frac{PYR_c}{K_pyruvate} * \left(1.0 + \frac{PYR_c}{K_pyruvate}\right)$$

43 “V_GPO” component

V_GPO_calculation

$$V_GPO = V_GPO_max * \frac{Gly_3_P_c}{K_Gly_3_P} * \left(1.0 + \frac{Gly_3_P_c}{K_Gly_3_P}\right)$$

44 “V_HK” component

V_HK_calculation

$$V_HK = V_HK_max * \frac{\frac{Glc_i}{K_Glc_i}}{\left(1.0 + \frac{Glc_i}{K_Glc_i} + \frac{Glc_6_P_g}{K_Glc_6_P_g}\right)} * \frac{\frac{ATP_g}{K_ATP}}{\left(1.0 + \frac{ATP_g}{K_ATP} + \frac{ADP_g}{K_ADP}\right)}$$

45 “V_GAPDH” component

V_GAPDH_calculation

$$V_GAPDH = V_GAPDH_max_plus * \frac{\frac{GA_3_P_g}{K_GA_3_P} * \left(\frac{NAD_g}{K_NAD} - V_GAPDH_max_ratio\right) * \frac{one_three_BPGA_g}{K_1.3_BPGA} * \frac{NADH_g}{K_NADH}}{\left(1.0 + \frac{GA_3_P_g}{K_GA_3_P} + \frac{one_three_BPGA_g}{K_1.3_BPGA}\right) * \left(1.0 + \frac{NAD_g}{K_NAD} + \frac{NADH_g}{K_NADH}\right)}$$

46 “V_PGK” component

V_PGK_calculation

$$V_PGK = V_PGK_max_plus * \frac{\frac{one_three_BPGA_g}{K_1.3_BPGA} * \left(\frac{ADP_g}{K_ADP} - V_PGK_max_ratio \right) * \frac{three_PGA}{K_3_PGA} * \frac{ATP_g}{K_ATP}}{\left(1.0 + \frac{one_three_BPGA_g}{K_1.3_BPGA} + \frac{three_PGA}{K_3_PGA} \right) * \left(1.0 + \frac{ADP_g}{K_ADP} + \frac{ATP_g}{K_ATP} \right)}$$

47 “V_GK” component

V_GK_calculation

$$V_GK = V_GK_max_plus * \frac{\frac{Gly_3_P_g}{K_Gly_3_P} * \left(\frac{ADP_g}{K_ADP} - V_GK_max_ratio \right) * \frac{glycerol_g}{K_glycerol} * \frac{ATP_g}{K_ATP}}{\left(1.0 + \frac{Gly_3_P_g}{K_Gly_3_P} + \frac{glycerol_g}{K_glycerol} \right) * \left(1.0 + \frac{ADP_g}{K_ADP} + \frac{ATP_g}{K_ATP} \right)}$$

48 “V_GDH” component

V_GDH_calculation

$$V_GDH = V_GDH_max_plus * \frac{\frac{DHAP_g}{K_DHAP} * \left(\frac{NADH_g}{K_NADH} - V_GDH_max_ratio \right) * \frac{Gly_3_P_g}{K_Gly_3_P} * \frac{NAD_g}{K_NAD}}{\left(1.0 + \frac{DHAP_g}{K_DHAP} + \frac{Gly_3_P_g}{K_Gly_3_P} \right) * \left(1.0 + \frac{NADH_g}{K_NADH} + \frac{NAD_g}{K_NAD} \right)}$$

49 “V_PFK” component

V_PFK_calculation

$$V_PFK = V_PFK_max * \frac{Ki_1}{(Fru_1.6_BP_g + Ki_1)} * \frac{\frac{Fru_6_P_g}{Km_Fru_6_P}}{\left(1.0 + \frac{Fru_6_P_g}{Km_Fru_6_P} + \frac{Fru_1.6_BP_g}{Ki_2} \right)} * \frac{\frac{ATP_g}{Km_ATP}}{\left(1.0 + \frac{ATP_g}{Km_ATP} \right)}$$

50 “V_PYK” component

V_PYK_calculation

$$V_PYK = V_PYK_max * \frac{\left(\frac{PEP_c}{Km_PEP} \right)^n}{\left(1.0 + \left(\frac{PEP_c}{Km_PEP} \right)^n \right)} * \frac{\frac{ADP_c}{Km_ADP}}{\left(1.0 + \frac{ADP_c}{Km_ADP} \right)}$$

Km_PEP_calculation

$$Km_PEP = 0.34 * \left(1.0 + \frac{ATP_c}{0.57} + \frac{ADP_c}{0.64} \right)$$

51 “V_ALD” component

V_ALD_calculation

$$V_{ALD} = V_{ALD_max_plus} * \frac{\left(\frac{Fru_{1.6_BP_g}}{Km_{Fru_{1.6_BP}}} - V_{ALD_max_ratio} * \frac{GA_{3_P_g}}{DHAP_g} * Km_{GA_{3_P}} * Km_{DHAP} \right)}{\left(1.0 + \frac{Fru_{1.6_BP_g}}{Km_{Fru_{1.6_BP}}} + \frac{GA_{3_P_g}}{Km_{GA_{3_P}}} + \frac{DHAP_g}{Km_{DHAP}} + \frac{Fru_{1.6_BP_g} * GA_{3_P_g}}{Km_{Fru_{1.6_BP}} * Ki_{GA_{3_P}}} + \frac{DHAP_g * GA_{3_P_g}}{Km_{DHAP} * Km_{GA_{3_P}}} \right)}$$

Km_Fru_1.6_BP_calculation

$$Km_{Fru_{1.6_BP}} = 9.0E - 3 * \left(1.0 + \frac{ATP_g}{0.68} + \frac{ADP_g}{1.51} + \frac{AMP_g}{3.65} \right)$$

52 “V_ATP_utilisation” component

V_ATP_utilisation_calculation

$$V_{ATP_utilisation} = k * \frac{ATP_c}{ADP_c}$$