SUPLEMMENTARY FILE I. COMPONENTS, CONSTANTS AND REACTIONS OF THE MODEL

The following pages include tables with all the components, reactions with their stoichiometry, physical constants and kinetic constants used in the model; and all the rate equations and differential equations employed in the model.

Table 1. Components of the model with the abbreviations used

Name of the component	Abbreviation (Reduced/Oxidized)
Neutral form of P680 (Photosystem II)	P680
Excited form of P680 (Photosystem II)	P680a
Protonated form of P680 (Photosystem II)	P680p
Q_A site of the Photosystem II	QA_r/QA_o
Non-reduced plastoquinol	PQ
Reduced plastoquinol	PQH2
ISP subunit of cytochrome b6f	ISP_r/ISP_o
$Heme_{bp}$ site of cytochrome b6f	hemebp_r/hemebp_o
$Heme_{bn}$ site of cytochrome b6f	hemebn_r/hemebn_o
Cytochrome f	cytf_r/cytf_o
Plastocyanin	PC_r/PC_o
Neutral form of P700 (Photosystem I)	P700
Excited form of P700 (Photosystem I)	P700a
Protonated form of P700 (Photosystem I)	P700p
A0 chlorophyll (Photosystem I)	A0_r/A0_o
Ferredoxin	Fd_r/Fd_o
Nicotinamide adenine dinucleotide phosphate	NADP
Reduced nicotinamide adenine dinucleotide phosphate	NADPH
Adenosine diphosphate	ADP
Inorganic phosphate	Pi
Adenosine triphosphate	ATP
Protons in the cytoplasm	H_c
Protons in the lumen	H_l
Gliceraldehyde-3-phosphate	G3P
Nitrate	NO3
Nitrite	NO2
Ammonia	NH3
Ion calcium	Ca2+
Ion chloride	Cl-
Ion potassium	K+
Ion magnesium	Mg2+
Oxygen	O2
Hydrogen	H2

Table 2. Reactions in the model, including abbreviation, stoichiometry and rate equation type used.

Reaction	Abb.	Stoichiometry	Equation
Water splitting at OEC	vWS	2 H2O+ 4 P680p -> 4 P680 +4 H_l + O2	MM
Excitation of P680	vP680_P680a	4 P680 + 4 photons -> 4 P680a	MM
Reversion of P680a	vP680a_P680	P680a -> P680	MAL
Reduction of QA	VP680a_QA	4 P680a + 4 QA(ox) <-> 4 P680p + 4 QA(r)	ER-HMM
Reduction of PQ	V2QAr_PQH2	2 QA(r) + 2 H_c + PQ< -> 2 QA(ox) + PQH2	ER-HMM
Reduction of ISP	vPQH2_ISP	PQH2 + ISP(o) <-> SPQ +ISP(r) +2 H(l)	ER-HMM
Reduction of hemebp	vSPQ_hemebp	SPQ + hemebp(o) -> PQ + hemebp(r)	-
Reduction of cytochrome f	vISP_cytf	ISP(r) + cytf(o)< -> ISP(o) + cytf(r)	ER-HMM
Reduction of PC	vcytf_PC	cytf(r) + PC(o) <-> PC(r) + cytf(o)	ER-HMM
Reduction of P700p	vPC_P700	PC(r) + P700p <-> PC(o) + P700	ER-HMM
Reduction of hemebn	vhemebbp_hemebn	hemebp(r) + hemebn(o) ->hemebp(r) + hemebn(o)	E-MM
Reduction of PQ (PQ cycle)	vhemebn_PQH2	2 hemebn(r) + PQ -> 2 hemebn(o) + PQH2	E-MM
Excitation of P700	vP700_P700a	P700 + photon -> P700a	MM
Reversion of P700a	vP700a_P700	P700a -> P700	MAL
Reduction of A0	vP700a_A0r	P700a + A0(o) <->	ER-HMM
Reduction of Ferredoxin	vA0r_Fdr	A0(r) + Fd(o) <-> A0(o) + Fd(o)	ER-HMM
Reduction of NADP	vFdr_NADPH	2 Fd(o) + NADP + H+(c) <-> 2 Fd(r) +NADPH	ER-HMM
ATP Synthesis	vADP_ATP	ADP + Pi + 4.67 H+(l) <-> ATP + 4.67 H+(c)	ATPModule
Short Cycle Around PSI (PGR5)	vFdr_PQH2	2 Fd(r) + PQ + 2 H+(s) <->	ER-HMM
Long Cycle Around PSI (NDH-1)	vNADPH_PQH2	NADPH + PQ <-> NADP + PQ	ER-HMM
G3P synthesis (C output)	vCO2_G3P	3 CO2 + 6 NADPH + 5 H20 + 9 ATP -> G3P + 2 H(c) + 6 NADP + 9 ADP + 8 Pi	E-MM
G3P output	vG3P_G3Pext	G3P -> G3Pext	MAL
Nitrate assimilation (N output)	vNO3ext_NO3	NO3ext + ATP + H2O -> NO3 +ADP +Pi	MAL
Nitrite assimilation (N output)	vNO2ext_NO2	NO2ext + ATP +H2O -> NO2 + ADP +Pi	MAL
Nitrate reduction	vNO3_NO2	NO3 + 2 Fd(r) + 2 H(c) -> NO2 + 2 Fd(o) +H2O	E-MM
Nitrite reduction	vNO2_NH3	NO2 + 6 Fd(r) + 7 H(c) -> NH3 + 6 Fd(o) + 2 H2O	E-MM
NH3 output	vNH3_NH3ext	NH3 -> NH3ext	MAL
Mehler reaction (Flv1-3)	vFlv1_3	4 Fd(r) + 4 H+(c) + O2 -> 4 Fd(o) + 2 H2O	E-MM
PC-mediated oxygen reduction (cyt c)	vPC_H2O	4 PC(r) + O2 + 8 H+(c) -> 4 PC(r) + 2 H2O + 4 H	E-MM
PQH2 mediated oxygen reduction (cyt bd)	vPQH2_H2O	2 PQH2 + O2 -> 2 PQ + 2 H2O	E-MM
O2 output	vO2_O2ext	O2 -> O2ext	MAL
Calcium flux across the membrane	vCa2flux	Ca2+(l) -> Ca2+(c)	Nernst-Planck
Chloride flux across the membrane	vClflux	Cl-(l) -> Cl-(c)	Nernst-Planck
Calcium flux across the membrane	vCa2flux	Ca2+(l) -> Ca2+(c)	Nernst-Planck
Potassium flux across the membrane	vKflux	K+(l) -> K+(c)	Nernst-Planck
Magnessium flux across the membrane	vMg2flux	Mg2+(l) -> Mg2+(c)	Nernst-Planck

NADPH-mediated H2 synthesis	vNADPH_H2	NADPH + 2 H+(c) -> NADP + H2	MM
Fd-mediated H2 synthesis	vFd_H2	2 Fd(r) + 2 H()	MM

Table 3. Physical constants used in the model

Constant	Definition	Value	Units
Vc	Volume of cytoplasm	0.75	ml
Vl	Volume of lumen	0.25	ml
F	Faraday constant	9.649·104	C·mol-1
HPR	Proton to ATP ratio	4.67	Dimensionless
ΔG°	ATP synthesis Gibbs standard free energy	28.1	kJ·mol-1
R	Molar gas constant	8.314	J·K-1·mol1
T	Temperature	298	K
C	Membrane capacitance	1	F
P	Membrane permeability	1	cm·s-1

Table 4. Midpoint redox potentials used in the model (Antal and Kovalenko, 2013)

Redox couple	Midpoint redox potential (mV)
P680a/P680p	-705
QA_o/QA_r	-30
PQ/PQH2	82
ISP_o/ISP_r	290
Cytf_o/Cytf_r	350
PC_o/PC_r	370
P700p/P700	440
P700a/P700p	-1300
A0_o/A0_r	-680
Fd_o/Fd_r	-440
NADP/NADPH	-320

Table 5. Initial concentration values of the components of the model. The values of these initial concentrations are set only for testing purposes, and have no biological relevance

Component	Initial Value
P680	0.1
P680a	0.1
P680p	100
QA_r	0.1
QA_o	100
PQ	100
PQH2	0.1
ISP_o	100
ISP_r	0.1

hemebp_o	100
hemebp_r	0.1
cytf_o	100
cytf_r	0.1
PC_o	100
PC_r	0.1
P700	0.1
P700p	100
P700a	0.1
hemebn_o	100
hemebn_r	0.1
A0_o	100
A0_r	0.1
Fd_o	100
Fd_r	0.1
NADP	100
NADPH	1
ADP	100
Pi	100
ATP	0.1
H_c	1*10-7
H_l	1*10-7
G3P	0.01
NO3	0.01
NO2	0.01
NH3	0.01
Ca2+_l	0.01
Ca2+_c	0.01
Cl-_l	0.01
Cl-_c	0.01
K+_l	0.01
K+_c	0.01
Mg2+_l	0.01
Mg2+_c	0.01
O2	0.0001
H2	0.0001

Table 6. Kinetic constants employed in the model. The values of these kinetic constants are set only for test purposes, and have no biological relevance.

Reaction	Kinetic constant	Value
vWS	vmax_ws	10
	kP680p_r1	0.1
vP680_P680a	Vmax_vP680_P680a	10
	kP680_P680a	0.9
vP680a_P680	kP680a_P680	0.1

vP680a_QA	vmax_vP680a_QA	10
	kP680a_r4	0.1
	kQAo_r4	0.1
	kP680p_r4	1
	kQAr_r4	1
v2QAr_PQH2	vmax_v2QAr_PQH2	10
	kQAr_r5	0.1
	kPQ_r5	0.1
	kQAo_r5	10
	kPQH2_r5	10
vPQH2_ISP	vmax_vPQH2_ISP	10
	kPQH2_r6	0.1
	kISPo_r6	0.1
	kPQ_r6	10
	kISPr_r6	10
vISP_cytf	Vmax_vISP_cytf	10
	kISPr_r8	0.1
	Kcytfo_r8	0.1
	kISPo_r8	10
	Kcytfr_r8	10
vcytf_PC	vmax_vcyf_PC	10
	Kcytfr_r9	0.1
	kPCo_r9	0.1
	Kcyfo_r9	10
	kPCr_r9	10
vPC_P700	vmax_vPC_p70	10
	kPCr_r10	0.1
	kP700p_r10	0.1
	kPCo_r10	10
	kP700_r10	10
vhemebp_hemebn	vmax_vhemebp_hemebn	10
	khemebpr_r11	0.1
	khemebno_r11	0.1
vhemebn_PQH2	vmax_vhemebn_PQH2	1
	khemebn_r12	0.1
	kPQ_r12	0.1
vP700_P700a	Vmax_vP700_P700a	10
	kP700_P700a	0.1
vP700a_P700	K_vP700a_P700	0.01
vP700a_A0r	vmax_vP700a_A0r	10
	kP700a_r15	0.1
	kA0_r15	0.1
	kP700p_r15	10
	kA0r_r15	10
vA0r_Fdr	Vmax_vA0r_Fdr	10
	kA0r_r16	0.1
	kFdo_r16	0.1
	kA0o_r16	10
	kFdr_r16	10
vFdr_NADPH	vmax_vFdr_NADPH	10

	kFdr_r17	0.1
	KNADP_r17	0.1
	kFdo_r17	10
	kNADPH_r17	10
vADP_ATP	vmax_vADP_ATP	10
	kADP_r18	0.1
	kPi_r18	0.1
	kATP_r18	0.1
vFdr_PQH2	vmax_vFdr_PQH2	1
	kFdr_r19	10
	kPQ_r19	10
	kFdo_r19	100
	kPQH2_r19	100
vNADPH_PQH2	vmax_vNADPH_PQH2	1
	kNADPH_r20	10
	kPQ_r20	10
	kNADP_r20	100
	kNPQH2_r20	100
vCO2_G3P	vmax_vCO2_G3P	1
	kNADPH_r21	0.1
	kATP_r21	0.1
vG3P_G3Pext	k_vG3p_G3Pext	1
vNO3ext_NO3	k_vNO3ext_NO3	0.1
vNO2ext_NO2	k_vNO2ext_NO2	0.01
vNO3_NO2	vmax_vNO3_NO2	1
	kNO3_r25	0.01
	kFdr_r25	0.1
vNO2_NH3	vmax_vNO2_NH3	1
	kNO2_r26	0.01
	kFdr_r26	0.1
vNH3_NH3ext	k_vNH3_NH3ext	1
vFlv1_3	vmax_vFlv1_3	1
	kFdr_r28	10
	kO2_r28	1
vPC_H2O	vmax_vPC_H2O	1
	kPCr_r29	10
	kO2_r29	1
vPQH2_H20	vmax_vPQH2_H2O	1
	kPQH2_r30	10
	kO2_r30	1
vO2_O2ext	k_vO2_O2ext	0.01
vNADPH_H2	vmax_vNADPH_H210	10
	kNADPH_r36	1000
vFd_H2	vmax_vFd_H2	10
	kFd_r37	10

Supplementary File II. Rate equations and differential equations of the model

The following pages include the rate equations and differential equations as they have been introduced in the model, including specific kinetic constants for every reaction

Rate Equations

$$vWS = \frac{v_{\max\_ws}[P680p]}{K_{P680p\_r1}+[P680p]} \tag{1}$$

$$vP680\_P680a = \frac{v_{\max\_vP680\_P680a}[P680]}{K_{P680\_P680a}+[P680]} \tag{2}$$

$$vP680\_P680a = kP680a\_P680 * [P680a] \tag{3}$$

$$vP680a\_QA = \frac{v_{\max\_vP680a\_QA}\frac{[P680a]}{kP680a\_r4}\frac{[QAo]}{kQAo\_r4}-\frac{1}{K_E}\frac{[P680p]}{kP680p\_r4}\frac{[QAr]}{kQAr\_r4}}{\left(1+\frac{[P680a]}{kP680a\_r4}+\frac{[P680p]}{kP680p\_r4}\right)*\left(1+\frac{[QAo]}{kQAo\_r4}+\frac{[QAr]}{kQAr\_r4}\right)} \tag{4}$$

$$v2QAr\_PQH2 = \frac{v_{\max\_v2QAr\_PQH2}\frac{[QAr]}{kQAr\_r5}\frac{[PQ]}{kPQ\_r5}-\frac{1}{K_E}\frac{[QAo]}{kQAo\_r5}\frac{[PQH2]}{kPQH2\_r5}}{\left(1+\frac{[QAr]}{kQAr\_r5}+\frac{[QAo]}{kQAo\_r5}\right)*\left(1+\frac{[PQ]}{kPQ\_r5}+\frac{[PQH2]}{kPQH2\_r5}\right)} \tag{5}$$

$$vPQH2\_ISP = \frac{v_{\max\_vPQH2\_ISP}\frac{[PQH2]}{kPQH2\_r6}\frac{[ISPo]}{kISPo\_r6}-\frac{1}{K_E}\frac{[PQ]}{kPQ\_r6}\frac{[ISPr]}{kISPr\_r6}}{\left(1+\frac{[PQH2]}{kPQH2\_r6}+\frac{[PQ]}{kPQ\_r6}\right)*\left(1+\frac{[ISPo]}{kISPo\_r6}+\frac{[ISPr]}{kISPr\_r6}\right)} \tag{6}$$

$$vSPQ\_hemebp = vPQH2\_ISP \tag{7}$$

$$vISP\_cytf = \frac{v_{\max\_vISP\_cytf}\frac{[ISPr]}{kISPr\_r8}\frac{[cytfo]}{kcytfo\_r8}-\frac{1}{K_E}\frac{[ISPo]}{kISPo\_r8}\frac{[cytfr]}{kcytfr\_r8}}{\left(1+\frac{[ISPr]}{kISPr\_r8}+\frac{[ISPo]}{kISPo\_r8}\right)*\left(1+\frac{[cytfo]}{kcytfo\_r8}+\frac{[cytfr]}{kcytfr\_r8}\right)} \tag{8}$$

$$vcytf\_PC = \frac{v_{\max\_vcytf\_PC}\frac{[cytfr]}{kcytfr\_r9}\frac{[PCo]}{kPCo\_r9}-\frac{1}{K_E}\frac{[cytfo]}{kcytfo\_r9}\frac{[PCr]}{kPCr\_r9}}{\left(1+\frac{[cytfr]}{kcytfr\_r9}+\frac{[cytfo]}{kcytfo\_r9}\right)*\left(1+\frac{[PCo]}{kPCo\_r9}+\frac{[PCr]}{kPCr\_r9}\right)} \tag{9}$$

$$vPC\_P700 = \frac{v_{\max\_PC\_P700}\frac{[PCr]}{kPCr\_r10}\frac{[P700p]}{kP700p\_r10}-\frac{1}{K_E}\frac{[PCo]}{kPCo\_r10}\frac{[P700]}{kP700\_r10}}{\left(1+\frac{[PCr]}{kPCr\_r10}+\frac{[PCo]}{kPCo\_r10}\right)*\left(1+\frac{[P700p]}{kP700p\_r10}+\frac{[P700]}{kP700\_r10}\right)} \tag{10}$$

$$vhemebp_{hemebn} = \frac{v_{\max\_hembebp\_hemebn}[hemebp_r][hemebn_o]}{\frac{1}{k_{hemebpr_{r11}}k_{hemebno_{r11}}}+\frac{[hemebp_r]}{k_{hemebno_{r11}}}+\frac{[hemebn_o]}{k_{hemebpr_{r11}}}+[hemebp_r][hemebn_o]} \tag{11}$$

$$vhemebn\_PQH2 = \frac{v_{\max\_vhemebn\_PQH2}[hemebn\_r][PQ]}{\frac{1}{k_{hemebnr\_r12}k_{PQ\_r12}}+\frac{[hemebn\_r]}{k_{PQ\_r12}}+\frac{[PQ]}{k_{hemebnr\_r12}}+[hemebn\_r][PQ]} \quad (12)$$

$$vP700\_P700a = \frac{v_{\max\_vP700\_P700a}[P700]}{K_{P680\_P680a}+[P700]} \quad (13)$$

$$vP700a_{P700} = k\_vP700a\_P700 * [P700a] \quad (14)$$

$$vP700a\_A0r = \frac{v_{max\_vP700a\_A0r}\frac{[P700a]}{kP700a\_r15}\frac{[A0o]}{kA0o\_r15}-\frac{1}{K_E}\frac{[P700p]}{kP700p\_r15}\frac{[A0r]}{kA0r\_r15}}{\left(1+\frac{[P700a]}{kP700a\_r15}+\frac{[P680p]}{kP680p\_r4}\right)*\left(1+\frac{[A0o]}{kA0o\_r15}+\frac{[A0r]}{kA0r\_r15}\right)} \quad (15)$$

$$vA0r\_Fdr = \frac{v_{max\_vA0r\_Fdr}\frac{[A0r]}{kA0r\_r16}\frac{[Fdo]}{kFdo\_r16}-\frac{1}{K_E}\frac{[A0o]}{kA0o\_r16}\frac{[Fdr]}{kFdr\_r16}}{\left(1+\frac{[A0r]}{kA0r\_r16}+\frac{[A0o]}{kA0o\_r16}\right)*\left(1+\frac{[Fdo]}{kFdo\_r16}+\frac{[Fdr]}{kFdr\_r16}\right)} \quad (16)$$

$$vFdr\_NADPH = \frac{v_{max\_vFdr\_NADPH}\frac{[Fdr]}{kFdr\_r17}\frac{[NADP]}{kNADP\_r17}-\frac{1}{K_E}\frac{[Fdo]}{kFdo\_r17}\frac{[NADPH]}{kNADPH\_r17}}{\left(1+\frac{[Fdr]}{kFdr\_r17}+\frac{[Fdo]}{kFdo\_r17}\right)*\left(1+\frac{[NADP]}{kNADP\_r17}+\frac{[NADPH]}{kNADPH\_r17}\right)} \quad (17)$$

$$vATP = \frac{vATP_{max}\left([ADP][Pi]-\frac{[ATP]}{kE}\right)}{(K_{mADP}K_{mPi})\left(1+\frac{[ADP]}{K_{mADP}}+\frac{[Pi]}{K_{mPi}}+\frac{[ATP]}{K_{mAtP}}+\frac{[ADP][Pi]}{K_{mADP}K_{mPi}}\right)} \quad (18)$$

$$kE = e^{\left(-\frac{\Delta G}{RT}\right)} \quad (19)$$

$$\Delta G = \Delta G^{\circ} + 0.592HPRln\left(\frac{[H_l]}{[H_s]}\right) + HPR\Delta\Psi \quad (20)$$

$$vFdr\_PQH2 = \frac{v_{max\_vFdr\_PQH2}\frac{[Fdr]}{kFdr\_r19}\frac{[PQ]}{kPQ\_r19}-\frac{1}{K_E}\frac{[Fdo]}{kFdo\_r19}\frac{[PQH2]}{kPQH2\_r19}}{\left(1+\frac{[Fdr]}{kFdr\_r19}+\frac{[Fdo]}{kFdo\_r19}\right)*\left(1+\frac{[PQ]}{kPQ\_r19}+\frac{[PQH2]}{kPQH2\_r19}\right)} \quad (21)$$

$$vNADPH\_PQH2 = \frac{v_{max\_vNADPH\_PQH2}\frac{[NADPH]}{kNADPH\_r20}\frac{[PQ]}{kPQ\_r20}-\frac{1}{K_E}\frac{[NADP]}{kNADP\_r20}\frac{[PQH2]}{kPQH2\_r20}}{\left(1+\frac{[NADPH]}{kNADPH\_r20}+\frac{[NADP]}{kNADP\_r20}\right)*\left(1+\frac{[PQ]}{kPQ\_r20}+\frac{[PQH2]}{kPQH2\_r20}\right)} \quad (22)$$

$$vCO2\_G3P = \frac{v_{\max\_vCO2\_G3P}[NADPH][ATP]}{\frac{1}{k_{NADPH\_r21}k_{ATP\_r21}}+\frac{[NADPH]}{k_{ATP\_r21}}+\frac{[ATP]}{k_{NADPH\_r21}}+[NADPH][ATP]} \quad (23)$$

$$vG3P\_G3Pext = k\_vG3P\_G3Pext * [G3P] \quad (24)$$

$$vNO3ext\_NO3 = k\_vNO3ext\_NO3 * [ATP] \quad (25)$$

$$vNO2ext\_NO3 = k\_vNO2ext\_NO2 * [ATP] \quad (26)$$

$$vNO3\_NO2 = \frac{v_{\max\_vNO3\_NO2}[NO3][Fdr]}{\frac{1}{k_{NO3\_r25}k_{Fdr\_r25}}+\frac{[NO3]}{k_{Fdr\_r25}}+\frac{[Fdr]}{k_{NO3\_r25}}+[NO3][Fdr]} \quad (27)$$

$$vNO2\_NH3 = \frac{v_{\max\_vNO2\_NH3}[NO2][Fdr]}{\frac{1}{k_{NO2\_r26}k_{Fdr\_r26}}+\frac{[NO2]}{k_{Fdr\_r26}}+\frac{[Fdr]}{k_{NO2\_r26}}+[NO2][Fdr]} \quad (28)$$

$$vNH3\_NH3ext = k\_vNH3\_NH3ext * [NH3] \quad (29)$$

$$vFlv1\_3 = \frac{v_{\max\_vFlv1\_3}[Fdr][O2]}{\frac{1}{k_{Fdr\_r28}k_{O2\_r28}} + \frac{[Fdr]}{k_{O2\_r28}} + \frac{[O2]}{k_{Fdr\_r28}} + [Fdr][O2]} \quad (30)$$

$$vPC\_H20 = \frac{v_{\max\_vPC\_H2O}[PCr][O2]}{\frac{1}{k_{Fdr\_r29}k_{O2\_r29}} + \frac{[PCr]}{k_{O2\_r29}} + \frac{[O2]}{k_{PC\_r29}} + [PCr][O2]} \quad (31)$$

$$vPQH2\_H20 = \frac{v_{\max\_vPQH2\_H2O}[PQH2][O2]}{\frac{1}{k_{PQH2\_r30}k_{O2\_r30}} + \frac{[PQH2]}{k_{O2\_r30}} + \frac{[O2]}{k_{PQH2\_r30}} + [PQH2][O2]} \quad (32)$$

$$vO2\_O2ext = k\_vO2\_O2ext * [O2] \quad (33)$$

$$vNADPH\_H2 = \frac{v_{\max\_vNADPH\_H2}[NADPH]}{K_{NADPH\_r36}\left(1+\frac{O_2}{kI_{O_2}}\right)+[NADPH]} \quad (34)$$

$$vFd\_H2 = \frac{v_{\max\_vFd\_H2}[Fdr]}{K_{Fd\_r37}\left(1+\frac{O_2}{kI_{O_2}}\right)+[Fdr]} \quad (35)$$

$$vCa2flux = P_{Ca2+}\frac{2F\Delta\Psi\left([Ca2+_l]-[Ca2+_c]e^{-\frac{2F\Delta\Psi}{RT}}\right)}{1-e^{-\frac{2F\Delta\Psi}{RT}}} \quad (36)$$

$$vClflux = P_{Cl-}\frac{-F\Delta\Psi\left([Cl-_l]-[Cl-_c]e^{-\frac{-F\Delta\Psi}{RT}}\right)}{1-e^{-\frac{-F\Delta\Psi}{RT}}} \quad (37)$$

$$vKflux = P_{K+}\frac{F\Delta\Psi\left([K+_l]-[K+_c]e^{-\frac{F\Delta\Psi}{RT}}\right)}{1-e^{-\frac{F\Delta\Psi}{RT}}} \quad (38)$$

$$vMg2flux = P_{Mg}\frac{2F\Delta\Psi\left([Mg2+_l]-[Mg2+_c]e^{-\frac{2F\Delta\Psi}{RT}}\right)}{1-e^{-\frac{2F\Delta\Psi}{RT}}} \quad (39)$$

$$NetCharge_l = V_lF(2[Ca2+]_l - [Cl-]_l + [K+]_l + 2[Mg2+]_l) \quad (40)$$

$$NetCharge_c = V_cF(2[Ca2+]_c - [Cl-]_c + [K+]_c + 2[Mg2+]_c) \quad (41)$$

$$\Delta\Psi = \frac{NetCharge_l - NetCharge_c}{C} \quad (42)$$

$$pH_c = -\log([H_c]) \quad (43)$$

$$pH_l = -\log([H_l]) \quad (44)$$

$$\Delta pH = pH_c - pH_l \quad (45)$$

Differential equations

$dP680 = 4vWS - 4vP680\_P680a + vP680a\_P680$ (1)

$dP680a = 4vP680\_P680a - 4vP680\_QA - vP680a\_P680$ (2)

$dP680p = -4vWS + 4vP680a\_QA$ (3)

$dQA_{ox} = -4vP680a\_QA + 2v2QAr\_PQH2$ (4)

$dQA_{r} = 4vP680a\_QA - 2v2QAr\_PQH2$ (5)

$dPQ = -v2QAr\_PQH2 + vPQH2\_ISP + 2vPQH2\_H2O - vFdr\_PQH2 - vhemebn\_PQH2$ (6)

$dPQH2 = v2QAr\_PQH2 - vPQH2\_ISP + vhemebn\_PQH2 - 2vPQH2\_H20 + vFdr\_PQH2 + vNADPH\_PQH2$ (7)

$dISP_{ox} = -vPQH2\_ISP + vISP\_cytf$ (8)

$dISP_{r} = vPQH2\_ISP - vISP\_cytf$ (9)

$dcytf_{ox} = vISP\_cytf - vcytf\_PC$ (10)

$dcytf_{r} = -vISP\_cytf + vcytf\_PC$ (11)

$dPC_{ox} = -vcytf\_PC + vPC\_P700$ (12)

$dPC_{r} = vcytf\_PC - vPC\_P700$ (13)

$dP700 = vPC\_P700 - vP700\_P700a + vP700a\_P700$ (14)

$dP700p = -vPC\_P700 + vP700a\_A0r$ (15)

$dP700a = vP700\_P700a - vP700\_A0r - vP700a\_P700$ (16)

$dhemebp_{ox} = -vSPQ\_hemebp + vhemebp\_hemebn$ (17)

$dhemebp_{r} = vSPQ\_hemebp - vhemebp\_hemebn$ (18)

$dhemebn_{ox} = -vhemebp\_hemebn + 2vhemebn\_PQH2$ (19)

$dhemebn_{r} = vhemebp\_hemebn - 2vhemebn\_PQH2$ (20)

$dA0_{ox} = -vP700\_A0r + vA0r\_Fdr$ (21)

$dA0_{r} = vP700\_A0r - vA0r\_Fdr$ (22)

$$dFd_{ox} = -vA0r\_Fdr + 2vFdr\_NADPH + 2vFdr\_PQH2 + 2vNO3\_NO2 + 6vNO2\_NH3 + 4vFlv1\_3 + 2vFd\_H2 \quad (23)$$

$$dFd_{r} = vA0r\_Fdr - 2vFdr\_NADPH - 2vFdr\_PQH2 - 2vNO3\_NO2 - 6vNO2\_NH3 - 4vFlv1\_3 - 2vFd\_H2 \quad (24)$$

$$dNADP = -vFdr\_NADPH + 6vCO2\_G3P + vNADPH\_PQH2 + vNADPH\_H2 \quad (25)$$

$$dNADPH = vFdr\_NADPH - 6vCO2\_G3P - vNADPH\_PQH2 - vNADPH\_H2 \quad (26)$$

$$dADP = -vADP\_ATP + 9vCO2\_G3P + vNO3\_NO3ext + vNO2ext\_NO2 \quad (27)$$

$$dPi = -vADP\_ATP + 9vCO2\_G3P + vNO3\_NO3ext + vNO2ext\_NO2 \quad (28)$$

$$dATP = vADP\_ATP - 9vCO2\_G3P - vNO3\_NO3ext - vNO2ext\_NO2 \quad (29)$$

$$dH_{l} = \frac{V_c}{V_l}(4vWS + 2vPQH2\_ISP - 4.67vADP\_ATP + 4vPC\_H2O \quad (30)$$

$$dH_{c} = -2v2QAr\_PQH2 - 2vhemebn\_PQH2 + 4.67vADP\_ATP - 2vNO3\_NO2 - 7vNO2\_NH3 - 4vFlv1\_3 - 8vPC\_H2O - 2vNADPH\_PQH2 \quad (31)$$

$$dG3P = vCO2\_G3P - vG3PG3Pext \quad (32)$$

$$dNO3 = vNO3ext\_NO3 - vNO3\_NO2 \quad (33)$$

$$dNO2 = vNO2ext\_NO2 - vNO2\_NH3 \quad (34)$$

$$dNH3 = vNO2\_NH3 - vNH3\_NH3ext \quad (35)$$

$$dCa2+_{l} = -vCa2flux\frac{V_c}{V_l} \quad (36)$$

$$dCa2+_{c} = vCa2flux \quad (37)$$

$$dCl-_{l} = -vClflux\frac{V_c}{V_l} \quad (38)$$

$$dCl-_{c} = vClflux \quad (39)$$

$$dK+_{l} = -vKflux\frac{V_c}{V_l} \quad (40)$$

$$dK+_{c} = vKflux \quad (41)$$

$$dMg2+_{l} = -vMg2flux\frac{V_c}{V_l} \quad (42)$$

$$dMg2+_{c} = -vMg2flux \quad (43)$$

$$dO2 = vWS - vFlv1\_3 - vPC\_H2O - vPQH2\_H2O - vO2\_O2ext \quad (44)$$

$$dH2 = vNADPH\_H2 + vFd\_H2 \quad (45)$$