Supplemental Data

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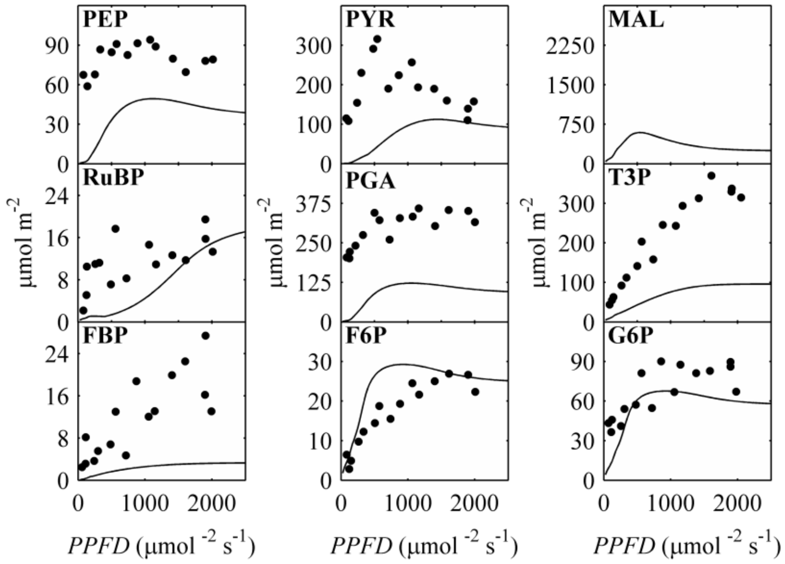
1. Supplemental Figures

1.1. Figure S1



Supplemental figure S1 Predicted changes in contents of key metabolites with changes in PPFD. As for Figure 3, but the response of metabolites to light. The intercellular CO_2 concentration (C_i) used in the simulation was 15 Pa.

1.2. Figure S2

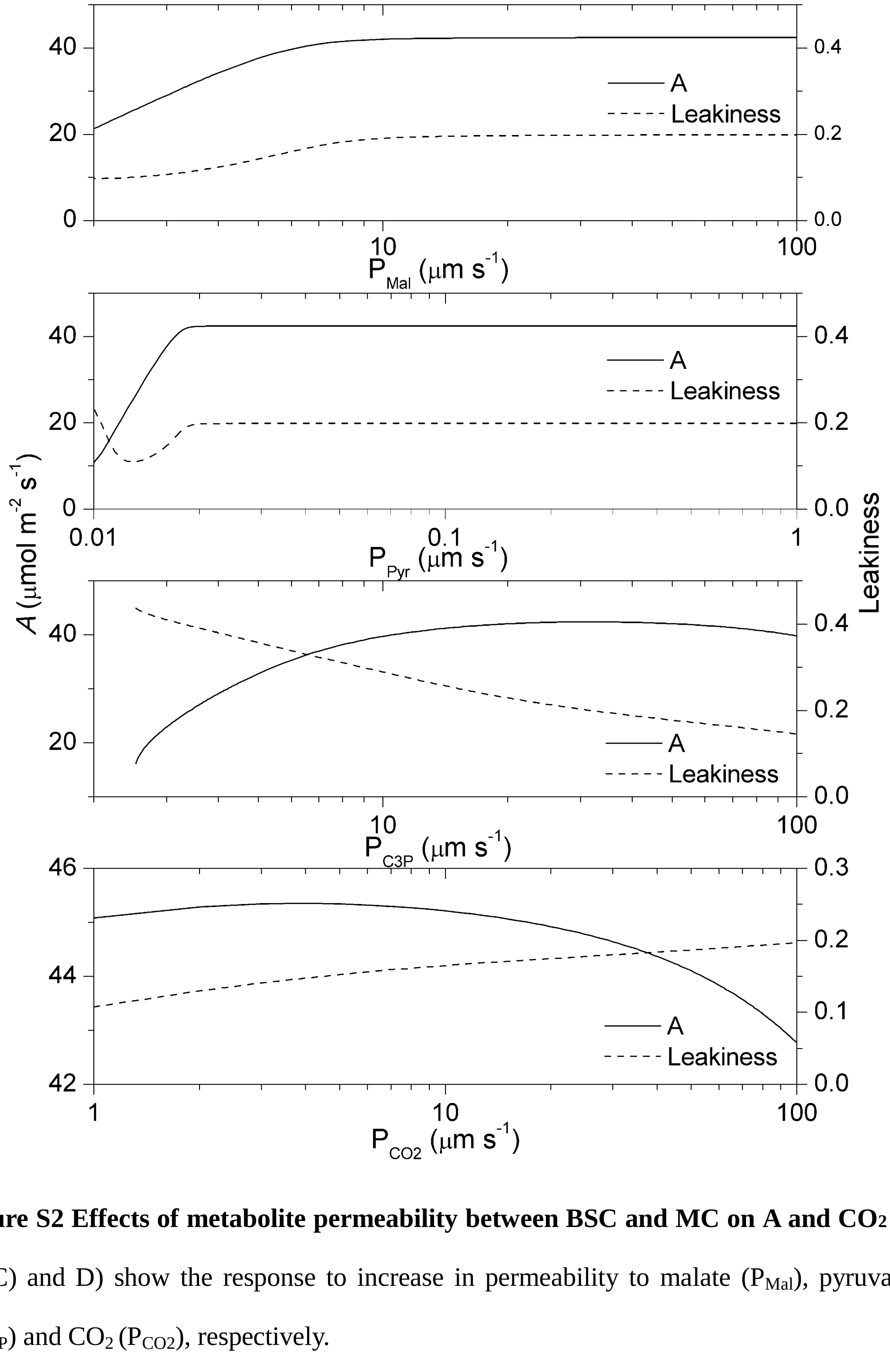


Figure S2 Effects of metabolite permeability between BSC and MC on A and CO_2 leakiness. A), B) C) and D) show the response to increase in permeability to malate (P_{Mal}), pyruvate (P_{Pyr}), C3P (P_{C3P}) and CO_2 (P_{CO2}), respectively.

1.3. Figure S3-S6

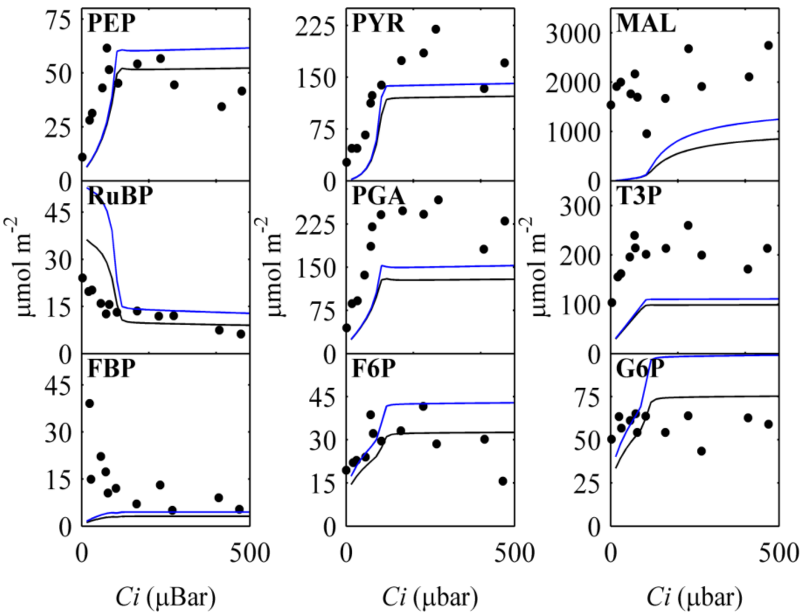


Figure S3 Phosphate concentration effects on steady-state contents of key metabolites of photosynthetic carbon metabolism. Blue lines represent the metabolite contents if increase phosphate concentration 20% in the model.

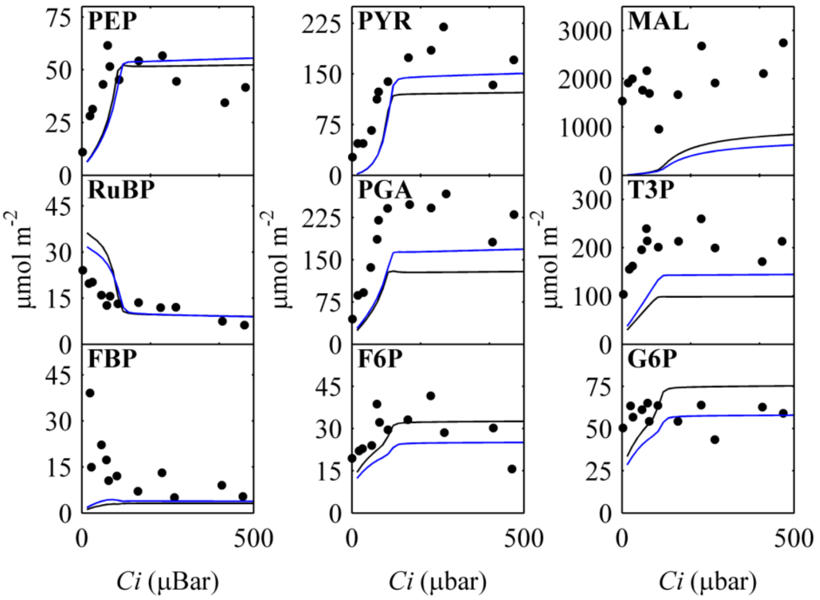


Figure S4 PGA and T3P related enzyme kinetic parameters effects on steady-state contents of key metabolites of photosynthetic carbon metabolism. Blue lines represent the metabolite contents if increase K_ms of PGA and T3P of related enzymes by 50%. PGA and T3P related enzyme means enzyme which use them as substrates or products.

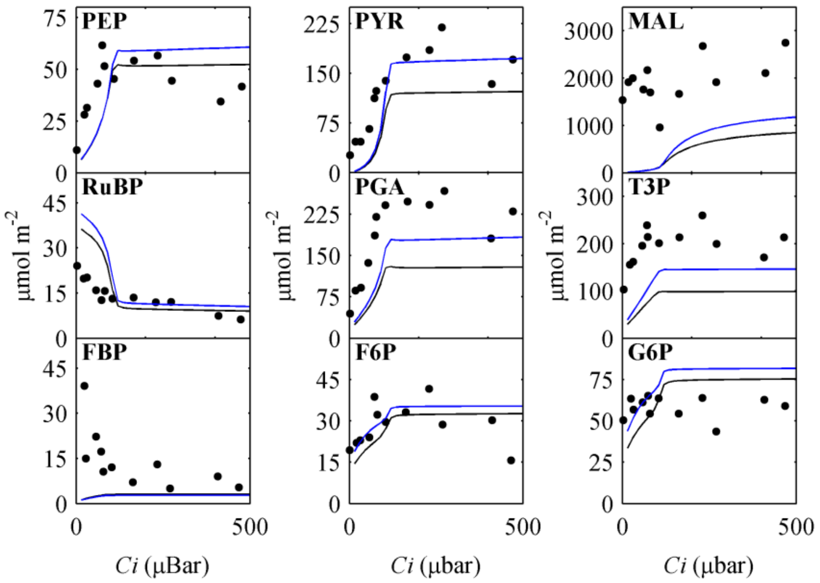


Figure S5 Phosphate concentration and enzyme kinetic parameters effects on key metabolites contents. Blue lines represent the metabolite contents if increase phosphate concentration 20% and K_ms of triose phosphates and PGA 50% together.

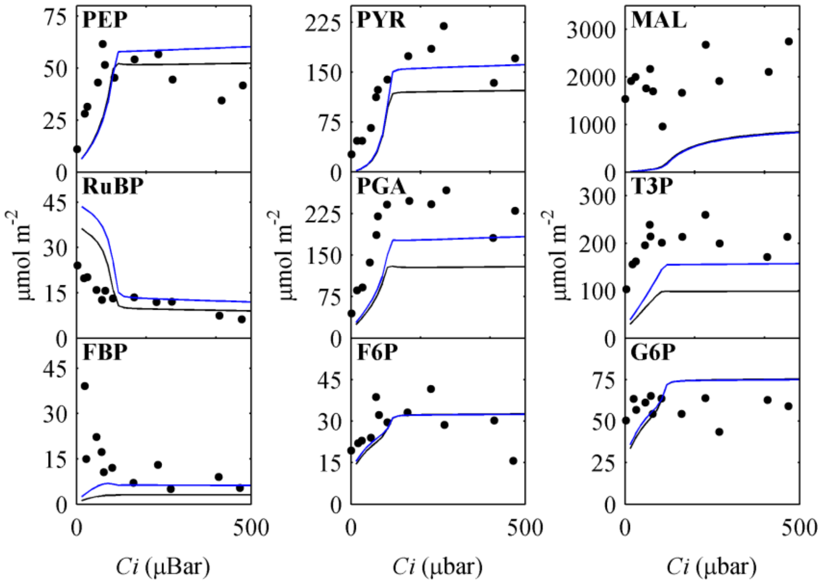


Figure S6 Cytolsolic FBPase enzyme kinetic parameters effects on key metabolites contents. Blue lines represent the metabolite contents with changed K_m of FBP of cytolsolic FBPase from 0.00108 to 0.05, in addition to modification of phosphate concentration, K_ms of triose phosphates and PGA

1.4. Figure S7

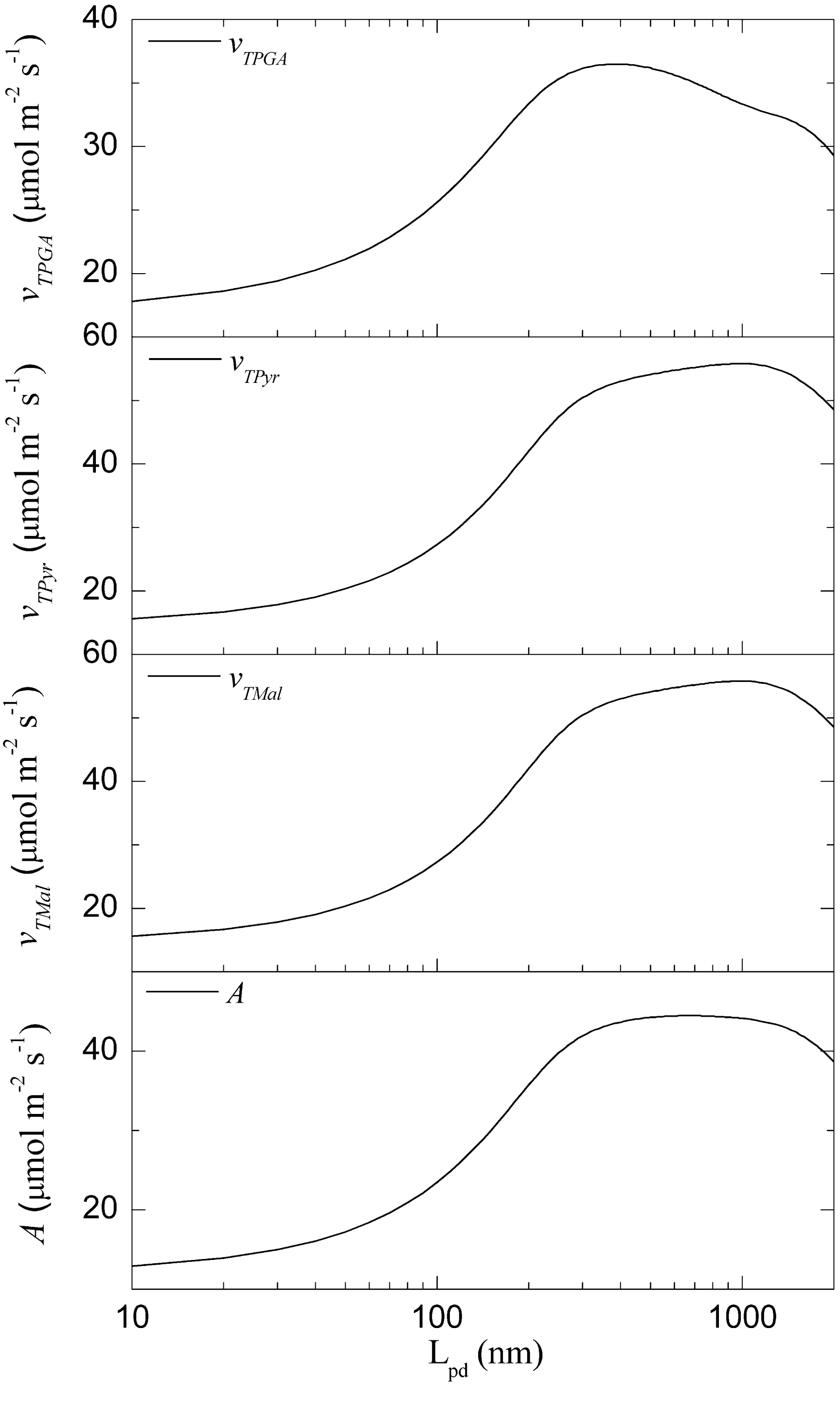


Figure S7 Effect of plasmodesmata length on *A* and metabolite fluxes between MCs and BSCs.

1.5. Figure S8

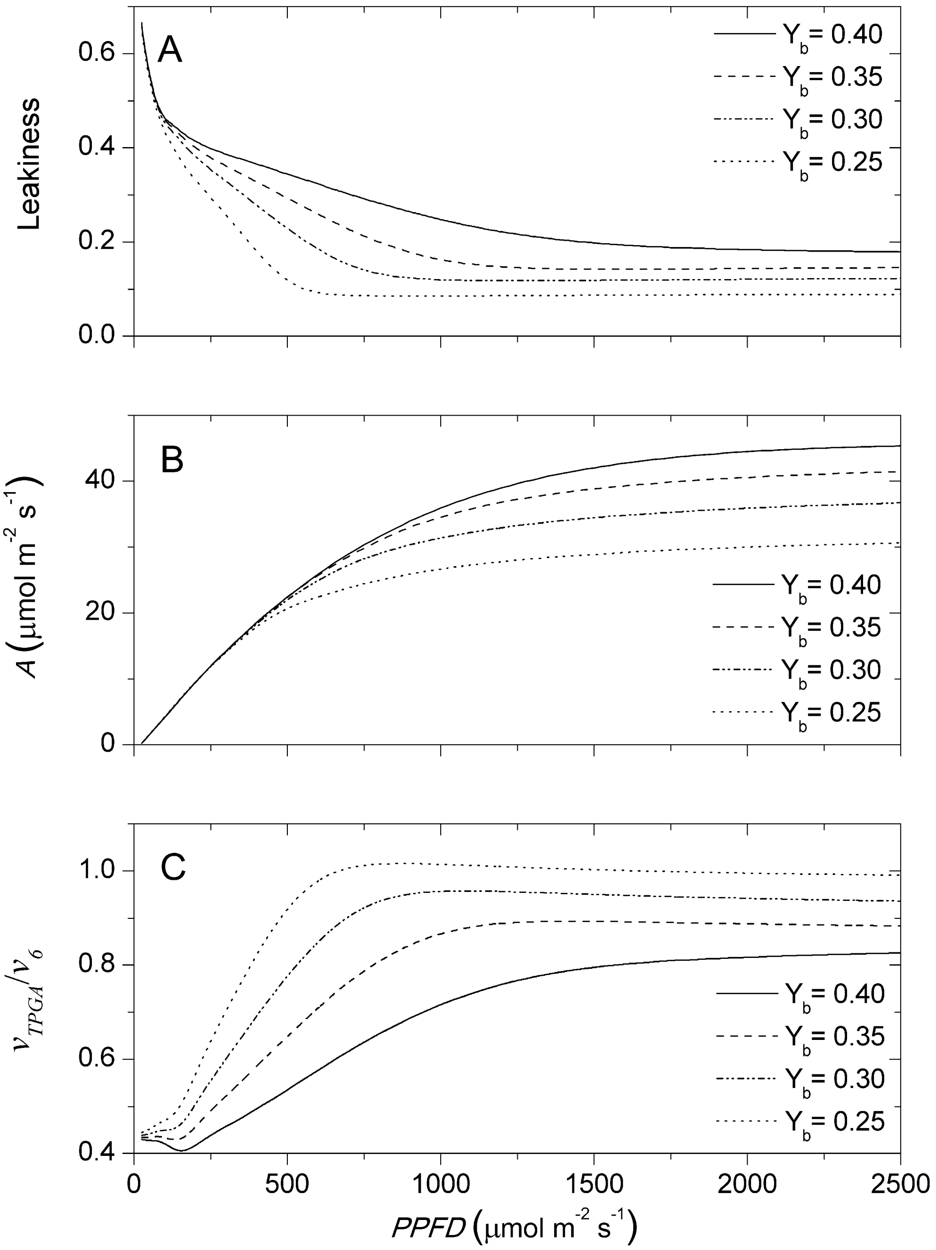


Figure S8 The proportion of J_{max_T} partitioned into BSC (Y_b) influences CO_2 leakiness, *A* and proportion of PGA transported to MCs. Here v_{TPGA} is the rate of PGA transport from BSC to MC and v_c is the rate of RuBP carboxylation.

1.6. Figure S9

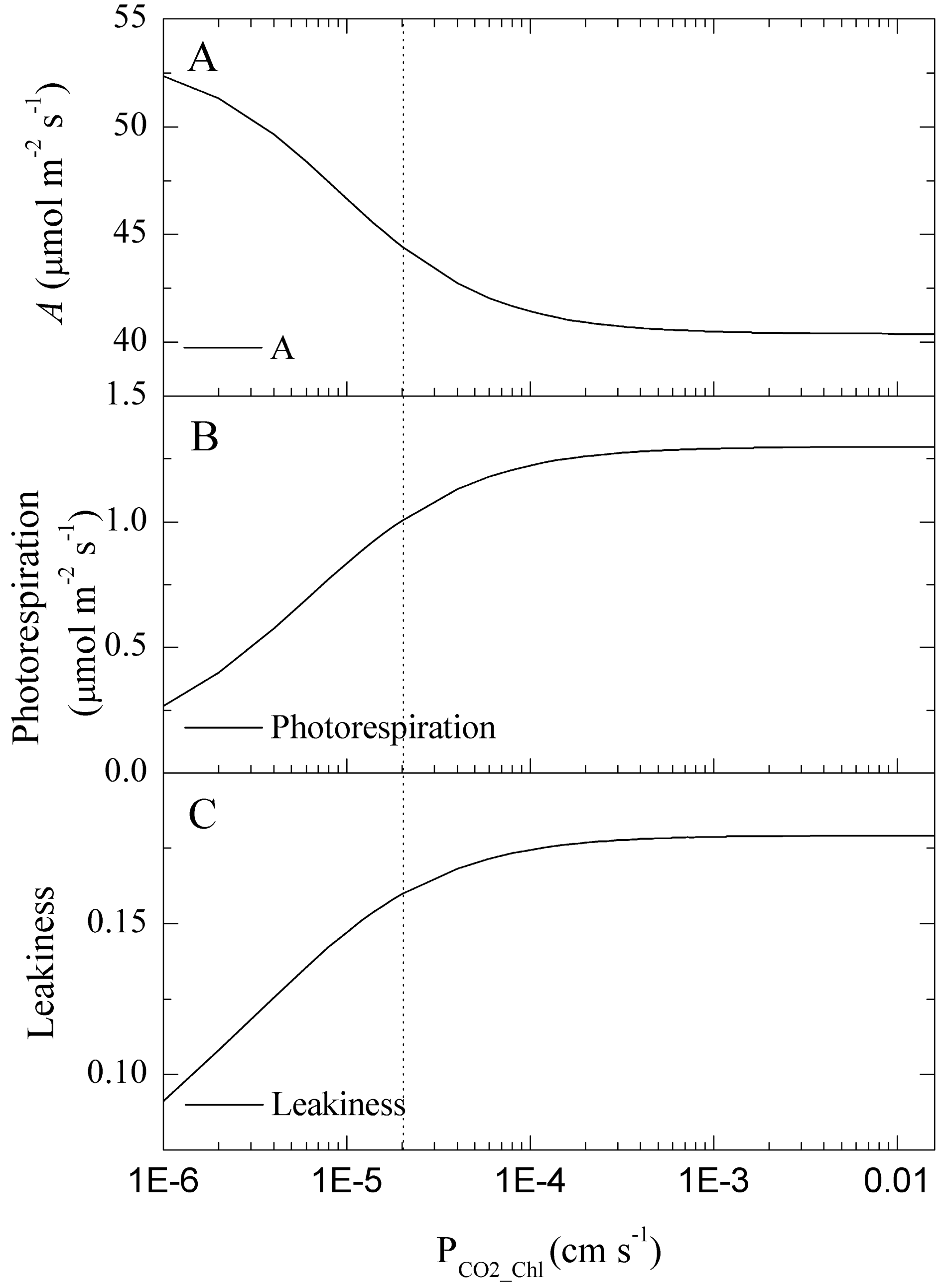


Figure S9 The effect of the chloroplast envelope permeability to CO_2 on photosynthesis, photorespiration and leakiness. (**A**) photosynthesis, (**B**) photorespiration and (**C**) leakiness. The dotted line represents the value used in the model.

2. Supplemental Tables

2.1 Table S1

Table S1 Photosynthetic flux control coefficients of enzymes and diffusion related parameters. We simulated the following scenarios: High light: *PPFD*=2000 μmol m^{-2} s^{-1}, C_i=15 Pa. Low light: *PPFD*=200 μmol m^{-2} s^{-1}, C_i =15 Pa. Low CO_2: *PPFD*=2000 μmol m^{-2} s^{-1}, C_i =5 Pa. Blue: the flux control coefficient of V_{max}, which decreased by 20%. During the calculation, V_{max} of other enzymes didn't change.

Abbreviation	EC Number or Legend	V_{max} (μmol m^{-2} s^{-1})	Flux Control Coefficient		
			High Light	Low CO_2	Low Light
CA	4.2.1.1	200000(160000)	0.001(0.001)	**0.185(0.221)**	0.000(0.000)
PEPC	4.1.1.31	170(136)	0.004**(0.128)**	**0.364(0.457)**	0.000(0.000)
NADP-MDH	1.1.1.82	90(72)	0.000(0.000)	0.000(0.000)	0.000(0.000)
NADP-ME	1.1.1.40	90(72)	0.002(0.014)	0.010(0.015)	0.000(0.000)
PPDK	2.7.9.1	90(72)	0.000(0.000)	0.000(0.000)	0.000(0.000)
Rubisco_CO_2	4.1.1.39	65(52)	**0.254(0.956)**	**0.099(0.157)**	**0.073(0.095)**
PGAK &GAPDH	2.7.2.3&1.2.1.13	225(180)	0.020**(0.399)**	0.001(0.003)	-0.005(0.000)
Aldolase	4.1.2.13FBP	58.5(46.8)	-0.020(-0.021)	-0.008(-0.011)	-0.005(-0.005)
FBPase	3.1.3.11	43.6(34.9)	0.004(0.017)	-0.009(-0.009)	-0.007(-0.006)
Aldolase	4.1.2.13SBP	109.7(87.8)	0.012(0.018)	0.000(0.000)	0.007(0.006)
SBPase	3.1.3.37	29.2(23.4)	**0.030(0.076)**	0.000(0.001)	0.010(0.014)
Transketolase	2.2.1.1X	281(224.8)	0.003(0.004)	0.000(0.000)	0.001(0.001)
Transketolase	2.2.1.1R	281(224.8)	0.000(0.001)	0.000(0.000)	0.000(0.001)
PRK	2.7.1.19	1170(936)	0.026**(0.040)**	0.000(0.000)	0.028**(0.033)**
PGAK_M &GAPDH_M	2.7.2.3M &1.2.1.13M	300(240)	0.002(0.036)	**-0.123(-0.102)**	0.009(0.011)
Rubisco_O_2	4.1.1.39	7.2(5.8)	-0.017(-0.014)	0.029(0.028)	**-0.063(-0.052)**
PGCAP	3.1.3.18	2621(2097)	0.000(0.000)	0.000(0.000)	0.000(0.000)
GO	1.1.3.15;	72.8(58.2)	0.000(0.000)	0.000(0.000)	0.000(0.000)
GGAT	2.6.1.4	137.3(109.8)	0.000(0.000)	0.000(0.000)	0.000(0.000)
Gly_ser	1.4.4.2&2.1.2.1	124.7(99.8)	0.000(0.000)	0.000(0.000)	0.000(0.000)
SGAT	2.6.1.45	165.3(132.2)	0.000(0.000)	0.000(0.000)	0.000(0.000)
HPR	1.1.1.29	500.5(400.4)	0.000(0.000)	0.000(0.000)	0.000(0.000)
GLYK	2.7.1.31	285.8(228.6)	0.000(0.000)	0.000(0.000)	0.000(0.000)
TGCA		300(240)	0.000(0.000)	0.000(0.000)	0.000(0.000)
TGCEA		250(200)	0.000(0.000)	0.000(0.000)	0.000(0.000)
Mutase& Enolase	5.4.2.1&4.2.1.11	1(0.8)	0.000(0.000)	0.000(0.000)	0.000(0.000)
Aldolase_M	4.1.2.13FBPM	8.0(6.4)	0.004(0.004)	0.017(0.019)	-0.001(-0.001)
FBPase_M	3.1.3.11M	6.4(5.1)	0.004(0.005)	0.017(0.018)	-0.001(-0.001)

UGPU	2.7.7.9	5.8(4.6)	0.001(0.001)	-0.006(-0.007)	0.000(0.000)
SPS	2.4.1.14	27.8(22.2)	0.001(0.001)	-0.020(-0.028)	0.000(0.000)
SPP	3.1.3.24	27.8(22.2)	0.000(0.000)	0.000(0.000)	0.000(0.000)
PFK	2.7.1.105	1.01(0.81)	-0.002(-0.002)	-0.013(-0.013)	0.000(0.000)
F26BPP	3.1.3.46	0.84(0.67)	0.002(0.002)	0.013(0.014)	0.000(0.000)
GPA	2.7.7.27	30(24)	0.002(0.051)	-0.003(-0.002)	-0.033(-0.025)
Diphosphatase	3.6.1.1	1000(800)	0.000(0.000)	0.000(0.000)	-0.001(-0.001)
Starch synthase	2.4.1.21	25(20)	0.000(0.001)	0.000(0.000)	0.000(0.000)
PGAsink	PGA Sink	2(1.6)	0.005(0.004)	-0.008(-0.006)	**0.037(0.033)**
ATPase	3.6.1.14M	300(240)	0.000(0.000)	0.000(0.000)	0.000(0.000)
FNR	1.18.1.2M	200(160)	0.000(0.000)	0.000(0.000)	0.000(0.000)
ATPase	3.6.1.14B	300(240)	0.000(0.000)	0.000(0.000)	0.000(0.000)
TPT	TPT_B	750(600)	0.000(0.001)	-0.004(-0.005)	0.001(0.001)
	TPT_M	750(600)	0.000(0.001)	-0.021(-0.024)	0.000(0.000)
DiT1	OAA_M	80(64)	0.000(0.000)	0.000(0.000)	0.000(0.000)
	MAL_B	150(120)	0.001(0.002)	0.019(0.024)	0.000(0.000)
DiT2	MAL_M	150(120)	0.000(0.000)	0.000(0.000)	0.000(0.000)
MEP	PYR_B	150(120)	0.001(0.002)	0.000(0.000)	0.000(0.000)
	PYR_M	150(120)	0.000(0.000)	0.000(0.000)	0.000(0.000)
PPT	PEP_M	150(120)	0.000(0.000)	0.000(0.000)	0.000(0.000)
J_{max}		500(400)	**0.600(0.790)**	-0.018**(-0.030)**	**0.074(0.099)**
I		2000 or 200	**0.134(0.219)**	-0.008(-0.012)	**0.969(1.057)**

Diffusion parameter	Value	Flux Control Coefficient		
		High light	Low CO_2	Low light
g_m	7(5.6) μmol m^{-2} s^{-1}Pa^{-1}	0.002(0.009)	**0.495(0.551)**	0.000(0.000)
D_{mal_PD}	6.77(5.42) ×10^{-10} m^2 s^{-1}	0.000(0.001)	**0.041(0.051)**	0.000(0.000)
D_{Pyr_PD}	7(5.6) ×10^{-10} m^2 s^{-1}	0.000(0.000)	0.000(0.000)	0.000(0.000)
D_{C3P_PD}	5.25(4.2) ×10^{-10} m^2 s^{-1}	0.000(0.006)	-0.020(-0.022)	0.002(0.003)
D_{co2_PD}	1.7(1.36) ×10^{-9} m^2 s^{-1}	**-0.045(-0.040)**	**-0.047(-0.043)**	**-0.042(-0.039)**
P_{co2_Bchl}	20(16) μm s^{-1}	-0.023(-0.024)	-0.004(-0.005)	-0.020(-0.022)
Φ	0.03(0.024)	**-0.045**(-0.028)	-0.028(-0.019)	**-0.040(-0.037)**
L_{pd}	400(320) nm	**0.044(0.065)**	0.028**(0.034)**	**0.040(0.043)**

2.2 Table S2

Table S2 Comparison of the impacts of using C3 and C4 homologs of enzymes related to C4 photosynthesis on *A* and nitrogen demand. Kinetic parameters for C3 and C4 homologs were used as inputs to the model to predict the CO$_2$ uptake rate under low and high CO$_2$ conditions. The CO$_2$ uptake ratio is ratio of CO$_2$ uptake rates predicted using kinetic parameters of a C3 homolog to that using a C4 homolog. Nitrogen cost for the synthesis of an enzyme was calculated based on the turnover number, molecular weight and the maximal rate of the enzyme. The nitrogen cost ratio was defined as the ratio of nitrogen required for synthesis of a C3 homolog to that for a C4 version.

PEPC (4.1.1.31)		**C$_4$ homolog**	**C$_3$ homolog**	**A Ratio (C$_3$/C$_4$)**	
Functional Parameters V$_{max}$=170 µmol m^{-2} s^{-1}	Km$_{PEP}$	1mM (Uedan, 1976)	0.069mM (De Nisi, 2000)	**C$_i$=5 Pa**	**C$_i$=15Pa**
	Km$_{HCO3}$	0.02mM (Uedan, 1976)	0.24mM (De Nisi, 2000)	**0.345**	**0.505**
	k$_{cat}$	66 s^{-1} (Xu, 2006)	69s^{-1} (Koizumi, 1996)	**Nitrogen Cost Ratio (C$_3$/C$_4$)**	
	MW	96000 (Harpster, 1986)	110000 (Koizumi, 1996)	**1.10**	

NADP-MDH (1.1.1.82)		**C$_4$ homolog**	**C$_3$ homolog**	**A Ratio (C$_3$/C$_4$)**	
Functional Parameters V$_{max}$=90 µmol m^{-2} s^{-1}	Km$_{NADPH}$	0.024mM (Kagawa, 1988)	0.039 mM (Fickenscher, 1983)	**C$_i$=5 Pa**	**C$_i$=15Pa**
	Km$_{OAA}$	0.056mM (Kagawa, 1988)	0.048 mM (Fickenscher, 1983)	**1**	**1**
	Km$_{NADP}$	0.073mM (Kagawa, 1988)	0.063 mM (Fickenscher, 1983)		
	Km$_{MAL}$	32mM (Kagawa, 1988)	0.0145mM (Fickenscher, 1983)		
	k$_{cat}$	677 s^{-1} (Kagawa, 1988)	118 s^{-1} (Fickenscher, 1983)	**Nitrogen Cost Ratio (C$_3$/C$_4$)**	
	MW	43000 (Agostino, 1992)	38500 (Fickenscher, 1983)	**5.14**	

Rubisco (4.1.1.39)		**C_4 homolog**	**C_3 homolog**	**A Ratio (C_3/C_4)**	
Functional Parameters V_{max}=65 μmol m^{-2} s^{-1}	Km_{CO2}	0.0162mM (Cousins, 2010)	0.0097mM (Cousins, 2010)	**C_i=5 Pa**	**C_i=15Pa**
	Km_{O2}	0.183mM (Cousins, 2010)	0.244mM (Cousins, 2010)	**1.033**	**1.026**
	k_{cat}	4.7 s^{-1} (Cousins, 2010)	3.8 s^{-1} (Cousins, 2010)	**Nitrogen Cost Ratio (C_3/C_4)**	
	MW	70000 (Spreitzer, 1999)	70000 (Spreitzer, 1999)	**1.24**	

NADP-ME (1.1.1.40)		**C_4 homolog**	**C_3 homologs**	**A Ratio (C_3/C_4)**	
Functional Parameters V_{max}=90 μmol m^{-2} s^{-1}	Km_{MAL}	0.23 mM (Detarsio, 2004)	2.96 mM $_{ME1}$ (Wheeler, 2008) 3.33 mM $_{ME2}$ (Wheeler, 2008) 0.83 mM $_{ME3}$ (Wheeler, 2008) **0.23 mM $_{ME4}$** (Wheeler, 2008)	**C_i=5 Pa**	**C_i=15Pa**
	Km_{NADPH}	0.045mM Ziegler (1974)	0.205 mM $_{ME1}$ (Wheeler, 2008) 0.0721mM $_{ME2}$ (Wheeler, 2008) 0.0065mM $_{ME3}$ (Wheeler, 2008) **0.0102mM $_{ME4}$** (Wheeler, 2008)	**0.926$_{ME1}$** **0.915$_{ME2}$** **0.975$_{ME3}$** **0.999$_{ME4}$**	**0.956$_{ME1}$** **0.936$_{ME2}$** **0.979$_{ME3}$** **0.998$_{ME4}$**
	Km_{pyr}	3mM (Ziegler , 1974)	16.9 mM $_{ME1}$ (Wheeler, 2008) 138.9 mM $_{ME2}$ (Wheeler, 2008) 48.2 mM $_{ME3}$ (Wheeler, 2008) **26.3 mM $_{ME4}$** (Wheeler, 2008)		
	k_{cat}	201.3s^{-1} (Detarsio,2003)	38.7s^{-1} $_{ME1}$ (Wheeler, 2008) 324.1 s^{-1} $_{ME2}$ (Wheeler, 2008) 268.1 s^{-1} $_{ME3}$ (Wheeler, 2008) **151.3 s^{-1} $_{ME4}$** (Wheeler, 2008)	**Nitrogen Cost Ratio (C_3/C_4)**	
	MW	62000 (Detarsio, 2004)	65000 (Wheeler, 2008)	**5.45 $_{ME1}$** **0.65 $_{ME2}$** **0.79 $_{ME3}$** **1.39 $_{ME4}$**	

PPDK (2.7.9.1)		**C_4 homolog**	**C_3 homolog**	**A Ratio (C_3/C_4)**	
Functional Parameters V_{max}=90 μmol m^{-2} s^{-1}	Km_{ATP}	0.082mM (Jenkins, 1985)	0.036mM (Meyer, 1978)	**C_i=5 Pa**	**C_i=15 Pa**
	Km_{PYR}	0.082mM Jenkins, 1985	0.025mM (Meyer, 1978)	**1**	**1**
	k_{cat}	6.02 s^{-1} McGuire, 1996	7.33s^{-1} (McGuire, 1996)	**Nitrogen Cost Ratio (C_3/C_4)**	
	MW	95000 Chastain, 2000	96600 (Moons, 1998)	**1.20**	

3. List of Abbreviations and Their Definitions

3.1 Metabolites

Abbreviation	Full Name	Units
ADPG	ADP-glucose	mM
CO_2	Carbon dioxide	mM
CA	Total adenylate nucleotide in the chloroplast stroma including ATP and ADP	mM
CN	Total of NADP+ and NADPH in chloroplast stroma	mM
CP	The total concentration of phosphate in chloroplast stroma	mM
DHAP	Dihydroxyacetone-phosphate	mM
DPGA	1,3-bisphosphoglycerate	mM
E4P	Erythrose 4-phosphate	mM
F26BP	Fructose 2,6–bisphosphate	mM
F6P	Fructose 6-phosphate	mM
FBP	Fructose 1,6–bisphosphate	mM
G1P	Glucose 1-phosphate	mM
G6P	Glucose 6-phosphate	mM
GAP	Glyceraldehyde 3-phosphate	mM
GCA	Glycollate	mM
GCEA	Glycerate	mM
GLU	Glutamate	mM
GLY	Glycine	mM
GOA	Glyoxylate	mM
HCO_3	Bicarbonate	mM
HexP	Hexose phosphate, includes F6P, G6P, and G1P	mM
HPR	Hydroxypyruvate	mM
KG	Ketoglutarate	mM
Mal	Malate	mM

O_2	Oxygen	mM
OAA	Oxaloacetate	mM
PEP	phosphoenolpyruvate	mM
PenP	Pentose phosphate including Ri5P, Ru5P, Xu5P	mM
PGA	3-Phosphoglycerate	mM
PGCA	3-Phosphoglycollate	mM
Pi	phosphate	mM
PPi	Pyrophosphate	mM
PYR	Pyruvate	mM
Ri5P	Ribose 5-phosphate	mM
Ru5P	Ribulose 5-phosphate	mM
RuBP	Ribulose 1,5-biphosphate	mM
S7P	Sedoheptulose 7-phosphate	mM
SBP	Sedoheptulose 1,7-bisphosphate	mM
SER	Serine	mM
SUC	Sucrose	mM
SUCP	Sucrose phosphate	mM
T3P	Triose phosphate including DHAP and GAP	mM
UDP	Uridine Diphosphate	mM
UDPG	Uridine Diphosphate Glucose	mM
UTP	Uridine Triphosphate	mM
Xu5P	Xylulose 5-phosphate	mM

3.2 Enzymes and Numbering

EC (or Model Defined)	Abbreviation	Full Name	Numbering in the Model
4.2.1.1	CA	Carbonic anhydrase	1
4.1.1.31	PEPC	Phosphoenolpyruvate carboxylase	2
2.7.9.1	PPDK	Pyruvate, phosphate dikinase	5
1.1.1.82	MDH	Malate dehydrogenase (NADP+)	3
1.1.1.40	ME	NADP-Malic enzyme	4
4.1.1.39	Rubisco	Ribulose-bisphosphate carboxylase	6
			Pr1
2.7.2.3	PGAK	Phosphoglycerate kinase	7
2.7.2.3M			7Mchl
1.2.1.13	GAPDH	Glyceraldehyde-3-phosphate	8
1.2.1.13M		dehydrogenase (NADP+)	8Mchl
5.3.1.1	T3PI	Triose-phosphate isomerase	9
4.1.2.13F	Aldolase	Fructose-bisphosphate aldolase	10
4.1.2.13S			12
4.1.2.13M			Suc1
3.1.3.37	SBPase	Sedoheptulose-bisphosphatase	13
3.1.3.11	FBPase	Fructose-bisphosphatase	11
3.1.3.11M			Suc2
2.2.1.1X	Transketolase	Transketolase	14
2.2.1.1R			15
5.3.1.6	Ri5PI	Ribose-5-phosphate isomerase	16
5.1.3.1	Ru5PE	Ribulose-phosphate 3-epimerase	17
2.7.1.19	PRK	Phosphoribulokinase	18
5.3.1.9	G6PI	Glucose-6-phosphate isomerase	Sta1
5.3.1.9M			Suc5
5.4.2.2	PGM	Phosphoglucomutase	Sta2

5.4.2.2M			Suc6
2.7.7.27	GPA	Glucose-1-phosphate adenylyltransferase	Sta3
3.6.1.1	Diphosphatase	inorganic diphosphatase	Sta4
2.4.1.21	Starch synthase	Starch synthase	Sta5
2.7.1.105M	PFK	6-phosphofructo-2-kinase	Suc3
3.1.3.46M	F26BPP	Fructose-2,6-bisphosphate 2-phosphatase	Suc4
2.7.7.9M	UGPU	UTP-glucose-1-phosphate uridylyltransferase	Suc7
2.4.1.14M	SPS	Sucrose-phosphate synthase	Suc8
3.1.3.24M	SPP	Sucrose-phosphate phosphatase	Suc9
3.1.3.18	PGCAP	Phosphoglycolate phosphatase	Pr2
1.1.3.15	GO	(S)-2-hydroxy-acid oxidase & Catalase(CAT, EC1.11.1.6)	Pr3
2.6.1.4	GGAT	Glycine transaminase	Pr4
2.6.1.45	SGAT	Serine-glyoxylate transaminase	Pr6
1.1.1.29	HPR	Glycerate dehydrogenase	Pr7
2.7.1.31	GLYK	Glycerate kinase	Pr8
3.6.1.14M	ATPase	ATP synthase	ATPM
3.6.1.14B			ATPB
1.18.1.2M	FNR	Ferredoxin-NADP+ reductase	NADPHM
PGASink	PGASink	PGA used for amino acid synthesis or other metabolic pathway	PGASink
Mutase& Enolase	Ex	5.4.2.1&4.2.1.11	Ex
Gly_ser	Gly_Ser	EC 1.4.4.2&EC2.1.2.1	Pr5
StarchDag	StarchDag	Starch degradation	StaDag

3.3 Metabolite Transport Process Through Chloroplast Membrane

Model Defined Numbering	Abbreviation	Full Name
$\mathbf{T_{PGAM}}$	TPT M	Triose phosphate translocator in mesophyll cell, which can transport PGA DHAP and GAP.
$\mathbf{T_{DHAPM}}$		
$\mathbf{T_{GAPM}}$		
$\mathbf{T_{PGAM}}$	TPT B	Triose phosphate translocator in bundle sheath cell
$\mathbf{T_{DHAPM}}$		
$\mathbf{T_{GAPM}}$		
$\mathbf{T_{OAAM}}$	DiT1	Dicarboxylate transporter
$\mathbf{T_{MALM}}$		
$\mathbf{T_{MALB}}$	DiT2	
$\mathbf{T_{PEPM}}$	PPT	PEP/phosphate translocator
$\mathbf{T_{PYRM}}$	MEPM	proton:pyruvate cotransporter

4 Equations

4.1 Rate Equations

4.1.1 CO$_2$ diffusion from air space to mesophyll cell.

$$v_{inf} = g_m \cdot \frac{1}{S_c} \cdot 10^{-3} \cdot (C_i - [CO_2]_{MC})$$

4.1.2 C4 cycle reactions

$$v_1 = \frac{V_{m\_1}\left(\cdot [CO_2]_{MC} - \frac{[HCO_3^-]_{MC} \cdot [H^+]_{MC}}{k_{e\_1}} \right)}{K_{mCO_2\_1} \cdot \left(1 + \frac{[CO_2]_{MC}}{K_{mCO_2\_1}} + \frac{[HCO_3^-]_{MC}}{K_{mHCO_3\_1}} \right)}$$

$$v_2 = \frac{V_{m\_2}\ \{HCO_3^-]_{MC} \cdot [PEP]_{MC}}{\left([PEP]_{MC} + K'_{mPEP\_2}\right)\left([HCO_3^-]_{MC} + K_{mHCO_3\_2}\right)}$$

$$K'_{mPEP\_2} = \frac{K_{mPEP\_2}\left(\cdot 1 + \frac{[MAL]_{MC}}{K_{iMAl\_2}}\right)}{\left(1 + \frac{[G6P]_{MC}}{K_{aG6P\_2}} + \frac{[T3P]_{MC}}{K_{aT3P\_2}}\right)}$$

$$v_3 = \frac{V_{m\_3}\left(\cdot [OAA]_{Mchl} \cdot [NADPH]_{Mchl} - \frac{[NADP]_{Mchl} \cdot [MAL]_{Mchl}}{k_{e\_3}}\right)}{K_{mOAA\_3} \cdot K_{mNADPH\_3}\ \alpha_3}$$

$$\alpha_3 = 1 + \frac{[OAA]_{Mchl}}{K_{mOAA\_3}} + \frac{[NADPH]_{Mchl}}{K_{mNADPH\_3}} + \frac{[NADP]_{Mchl}}{K_{mNADP\_3}} + \frac{[MAl]_{Mchl}}{K_{mMAl\_3}} + \\ + \frac{[OAA]_{Mchl} \cdot [NADPH]_{Mchl}}{K_{mOAA\_3} \cdot K_{mNADPH\_3}} + \frac{[NADP]_{Mchl} \cdot [MAl]_{Mchl}}{K_{mNADP\_3} \cdot K_{mMAl\_3}}$$

$$v_4 = \frac{V_{m\_4}\left(\cdot [MAl]_{Bchl} \cdot [NADP]_{Bchl} - \frac{[PYR]_{Bchl} \cdot [NADPH]_{Bchl} \cdot [CO_2]_{Bchl}}{k_{e\_4}}\right)}{K_{mMAL\_4} \cdot K_{mNADP\_4}\ \alpha_4}$$

$$\alpha_4 = 1 + \frac{[MAl]_{Bchl}}{K_{mMAL\_4}} + \frac{[NADP]_{Bchl}}{K_{mNADP\_4}} + \frac{[PYR]_{Bchl}}{K_{mPYR\_4}} + \frac{[NADPH]_{Bchl}}{K_{mNADPH\_4}} + \frac{[CO_2]_{Bchl}}{K_{mCO_2\_4}} + \\ + \frac{[MAl]_{Bchl} \cdot [NADP]_{Bchl}}{K_{mMAL\_4} \cdot K_{mNADP\_4}} + \frac{[PYR]_{Bchl} \cdot [NADPH]_{Bchl}}{K_{mPYR\_4} \cdot K_{mNADPH\_4}} + \frac{[PYR]_{Bchl} \cdot [CO_2]_{Bchl}}{K_{mPYR\_4} \cdot K_{mCO_2\_4}} + \\ + \frac{[CO_2]_{Bchl} \cdot [NADPH]_{Bchl}}{K_{mCO_2\_4} \cdot K_{mNADPH\_4}} + \frac{[PYR]_{Bchl} \cdot [NADPH]_{Bchl} \cdot [CO_2]_{Bchl}}{K_{mPYR\_4} \cdot K_{mNADPH\_4} \cdot K_{mCO_2\_4}}$$

$$v_5 = \frac{V_{m\_5}\ [PYR]_{Mchl} \cdot [ATP]_{Mchl}}{\left([PYR]_{Mchl} + K_{mPYR\_5} \cdot \left(1 + \frac{[PEP]_{Mchl}}{K_{iPEP\_5}}\right)\right)\left([ATP]_{Mchl} + K_{mATP\_5}\right)}$$

4.1.3 Calvin Cycle reactions

$$v_6 = \frac{V_{m\_6}\ \min\left(1, \frac{[RuBP]_{Bchl}}{[Rubisco]_{Bchl}}\right)\cdot [RuBP]_{Bchl}\cdot [CO_2]_{Bchl}}{\left([CO_2]_{Bchl} + K'_{mCO_2\_6}\right)\left([RuBP]_{Bchl} + K'_{mRuBP\_6}\right)}$$

$$K'_{mCO_2\_6} = K_{mCO_2\_6}\left(\cdot 1 + \frac{[O_2]_{Bchl}}{K_{iO_2\_6}}\right)$$

$$K'_{mRuBP\_6} = K_{mRuBP\_6}\left(\cdot 1 + \frac{[PGA]_{Bchl}}{K_{iPGA\_6}} + \frac{[FBP]_{Bchl}}{K_{iFBP\_6}} + \frac{[SBP]_{Bchl}}{K_{iSBP\_6}} + \frac{[Pi]_{Bchl}}{K_{iPi\_6}} + \frac{[NADPH]_{Bchl}}{K_{iNADPH\_6}}\right)$$

$$v_7 = \frac{V_{m\_7}\ \{[PGA]_{Bchl}\cdot [ATP]_{Bchl}}{\left([PGA]_{Bchl} + K_{mPGA\_7}\right)\left([ATP]_{Bchl} + K_{mATP\_7}\cdot(1 + \frac{[ADP]_{Bchl}}{K_{iADP\_7}})\right)}$$

$$v_8 = \frac{V_{m\_8}\ \{[DPGA]_{Bchl}\cdot [NADPH]_{Bchl}}{\left([DPGA]_{Bchl} + K_{mPGA\_8}\right)\left([NADPH]_{Bchl} + K_{mNADPH\_8}\right)}$$

$$v_{10} = \frac{V_{m\_10}\left(\cdot [GAP]_{Bchl}\cdot [DHAP]_{Bchl} - \frac{[FBP]_{Bchl}}{k_{e\_10}}\right)}{K_{mGAP\_10}\ K_{mDHAP\_10}\ \alpha_{10}}$$

$$\alpha_{10} = 1 + \frac{[GAP]_{Bchl}}{K_{mGAP\_10}} + \frac{[DHAP]_{Bchl}}{K_{mDHAP\_10}} + \frac{[FBP]_{Bchl}}{K_{mFBP\_10}} + \frac{[GAP]_{Bchl}\cdot [DHAP]_{Bchl}}{K_{mGAP\_10}\ K_{mDHAP\_10}}$$

$$v_{11} = \frac{V_{m\_11}\left(\cdot [FBP]_{Bchl} - \frac{[F6P]_{Bchl}\cdot [Pi]_{Bchl}}{k_{e\_11}}\right)}{\left([FBP]_{Bchl} + K_{mFBP\_11}\cdot\left(1 + \frac{[F6P]_{Bchl}}{K_{iF6P\_11}} + \frac{[Pi]_{Bchl}}{K_{iPi\_11}}\right)\right)}$$

$$v_{12} = \frac{V_{m\_12}\left(\cdot [DHAP]_{Bchl}\cdot [E4P]_{Bchl} - \frac{[SBP]_{Bchl}}{k_{e\_12}}\right)}{\left([DHAP]_{Bchl} + K_{mDHAP\_12}\right)\left([E4P]_{Bchl} + K_{mE4P\_12}\right)}$$

$$v_{13} = \frac{V_{m\_13}\left(\cdot[SBP]_{Bchl} - \frac{[Pi]_{Bchl}\cdot[S7P]_{Bchl}}{k_{e\_13}}\right)}{\left([SBP]_{Bchl} + K_{mSBP\_13}\cdot\left(1+\frac{[Pi]_{Bchl}}{K_{iPi\_13}}\right)\right)}$$

$$v_{14} = \frac{V_{m\_14}\left(\cdot[F6P]_{Bchl}\cdot[GAP]_{Bchl} - \frac{[Xu5P]_{Bchl}\cdot[E4P]_{Bchl}}{k_{e\_14}}\right)}{\left([F6P]_{Bchl} + K'_{mF6P\_14}\right)\left([GAP]_{Bchl} + K_{mGAP\_14}\right)}$$

$$K'_{mF6P\_14} = K_{mF6P\_14}\left(\cdot 1+\frac{[Xu5P]_{Bchl}}{K_{iXu5P\_14}}+\frac{[E4P]_{Bchl}}{K_{iE4P\_14}}\right)$$

$$v_{15} = \frac{V_{m\_15}\left(\cdot[GAP]_{Bchl}\cdot[S7P]_{Bchl} - \frac{[Ri5P]_{Bchl}\cdot[Xu5P]_{Bchl}}{k_{e\_15}}\right)}{\left([GAP]_{Bchl} + K'_{mGAP\_15}\right)\left([S7P]_{Bchl} + K_{mS7P\_15}\right)}$$

$$K'_{mGAP\_15} = K_{mGAP\_15}\left(\cdot 1+\frac{[Xu5P]_{Bchl}}{K_{iXu5P\_14}}+\frac{[Ri5P]_{Bchl}}{K_{iRi5P\_15}}\right)$$

$$v_{18} = \frac{V_{m\_18}\left(\cdot[ATP]_{Bchl}\cdot[Ru5P]_{Bchl} - \frac{[ADP]_{Bchl}\cdot[RuBP]_{Bchl}}{k_{e\_18}}\right)}{\left([ATP]_{Bchl} + K'_{mATP\_18}\right)\left([Ru5P]_{Bchl} + K'_{mRu5P\_18}\right)}$$

$$K'_{mATP\_18} = K_{mATP\_18}\left(\cdot 1+\frac{[ADP]_{Bchl}}{K_{iADP\_18}}\right)$$

$$K'_{mRu5P\_18} = K_{mRu5P\_18}\left(\cdot 1+\frac{[PGA]_{Bchl}}{K_{iPGA\_18}}+\frac{[RuBP]_{Bchl}}{K_{iRuBP\_18}}+\frac{[Pi]_{Bchl}}{K_{iPi\_18}}\right)$$

$$v_{7M} = \frac{V_{m\_7M}\left([PGA]_{Mchl}\cdot[ATP]_{Mchl}\right)}{\left([PGA]_{Mchl} + K_{mPGA\_7M}\right)\left([ATP]_{Mchl} + K_{mATP\_7M}\cdot\left(1+\frac{[ADP]_{Mchl}}{K_{iADP\_7M}}\right)\right)}$$

$$v_{8M} = \frac{V_{m\_8M}\ \{[DPGA]_{Mchl}\cdot[NADPH]_{Mchl}}{\left([DPGA]_{Mchl} + K_{mPGA\_8M}\right)\left([NADPH]_{Mchl} + K_{mNADPH\_8M}\right)}$$

4.1.4 Starch synthesis reactions

$$v_{Sta3}=\frac{V'_{m\_Sta3}\cdot\left([G1P]_{Bchl}\cdot[ATP]_{Bchl}-\frac{[ADPG]_{Bchl}\cdot[PPi]_{Bchl}}{K_{e\_Sta3}}\right)}{K_{mG1P\_Sta3}\cdot K'_{mATP\_Sta3}\cdot\alpha_{Sta3}}$$

$$V'_{m\_Sta3}=V_{m\_Sta3}\cdot\frac{[PGA]_{Bchl}}{\left([PGA]_{Bchl}+K_{aPGA\_Sta3}\right)}$$

$$K'_{mATP\_Sta3}=K_{mATP\_Sta3}\cdot\left(1+\frac{[ADP]_{Bchl}}{K_{iAADP\_ATP\_Sta3}}+\frac{[PPi]_{Bchl}}{K_{iCPPi\_ATP\_Sta3}}+\frac{[Pi]_{Bchl}}{K_{iAPi\_ATP\_Sta3}}\right)$$

$$\alpha_{\mathrm{Sta3}}=1+\frac{[G1P]_{Bchl}}{K_{mG1P\_Sta3}}+\frac{[ATP]_{Bchl}}{K'_{mATP\_Sta3}}+\frac{[ADPG]_{Bchl}}{K_{mADPG\_Sta3}}+\frac{[PPi]_{Bchl}}{K_{mPP1\_Sta3}}+$$
$$+\frac{[G1P]_{Bchl}\cdot[ATP]_{Bchl}}{\left(K_{mG1P\_Sta3}\cdot K'_{mATP\_Sta3}\right)}+\frac{[ADPG]_{Bchl}\cdot[PPi]_{Bchl}}{\left(K_{mADPG\_Sta3}\cdot K_{mPP1\_Sta3}\right)}$$

$$v_{Sta4}=\frac{V_{m\_Sta4}\cdot\left([PPi]_{Bchl}-\frac{[PPi]^2_{Bchl}}{K_{e\_Sta4}}\right)}{[PPi]_{Bchl}+K_{mPPi\_Sta4}}$$

$$v_{Sta5}=\frac{V_{m\_Sta5}\cdot[ADPG]_{Bchl}}{\left([ADPG]_{Bchl}+K_{mADPG\_Sta5}\right)}$$

4.1.5 Sucrose synthesis reactions

$$v_{Suc1}=\frac{V_{m\_Suc1}\left(\cdot[GAP]_{MC}\cdot[DHAP]_{MC}-\frac{[FBP]_{MC}}{k_{e\_Suc1}}\right)}{K_{mGAP\_Suc1}\,K_{mDHAP\_Suc1}\,\alpha_{Suc1}}$$

$$\alpha_{Suc1}=1+\frac{[GAP]_{MC}}{K_{mGAP\_Suc1}}+\frac{[DHAP]_{MC}}{K_{mDHAP\_Suc1}}+\frac{[FBP]_{MC}}{K_{mFBP\_Suc1}}+\frac{[GAP]_{MC}\cdot[DHAP]_{MC}}{K_{mGAP\_Suc1}\cdot K_{mDHAP\_Suc1}}$$

$$v_{Suc2}=\frac{V_{m\_Suc2}\left(\cdot[FBP]_{MC}-\frac{[F6P]_{MC}\cdot[Pi]_{MC}}{k_{e\_Suc2}}\right)}{K'_{mFBP\_Suc2}\;\alpha_{Suc2}}$$

$$\alpha_{Suc2}=1+\frac{[FBP]_{MC}}{K'_{mFBP\_Suc2}}+\frac{[F6P]_{MC}}{K_{mF6P\_Suc2}}+\frac{[Pi]_{MC}}{K_{mPi\_Suc2}}+\frac{[F6P]_{MC}\cdot[Pi]_{MC}}{K_{mF6P\_Suc2}\;K_{mPi\_Suc2}}$$

$$K'_{mFBP\_Suc2}=K_{mFBP\_Suc2}\left(\cdot 1+\frac{[F26BP]_{MC}}{K_{iF26BP\_Suc2}}\right)$$

$$v_{Suc3}=\frac{V_{m\_Suc3}\left(\cdot[ATP]_{MC}\cdot[F6P]_{MC}-\frac{[ADP]_{MC}\cdot[F26BP]_{MC}}{k_{e\_Suc3}}\right)}{\left([ATP]_{MC}+K'_{mATP\_Suc3}\right)\left([F6P]_{MC}+K'_{mF6P\_Suc3}\right)}$$

$$K'_{mATP\_Suc3}=K_{mATP\_Suc3}\left(\cdot 1+\frac{[ADP]_{MC}}{K_{iADP\_Suc3}}\right)$$

$$K'_{mF6P\_Suc3}=K_{mF6P\_Suc3}\left(\cdot 1+\frac{[F26BP]_{MC}}{K_{iF26BP\_Suc3}}\right)\cdot\left(1+\frac{[DHAP]_{MC}}{K_{iDHAP\_Suc3}}\right)$$

$$v_{Suc4}=\frac{V_{m\_Suc4}\cdot[F26BP]_{MC}}{K_{mF26BP\_Suc4}\left(\cdot 1+\frac{[F26BP]_{MC}}{K_{mF26BP\_Suc4}}\right)\left(1+\frac{[Pi]_{MC}}{K_{mPi\_Suc4}}\right)\left(1+\frac{[F6P]_{MC}}{K_{mF6P\_Suc4}}\right)}$$

$$v_{Suc7}=\frac{V_{m\_Suc7}\left(\cdot[UTP]_{MC}\cdot[G1P]_{MC}-\frac{[UDPG]_{MC}\cdot[PPi]_{MC}}{k_{e\_Suc7}}\right)}{K_{mUTP\_Suc7}\;K_{mG1P\_Suc7}\;\alpha_{Suc7}}$$

$$\begin{aligned}\alpha_{Suc7}=1&+\frac{[UTP]_{MC}}{K_{mUTP\_Suc7}}+\frac{[G1P]_{MC}}{K_{mG1P\_Suc7}}+\frac{[UDPG]_{MC}}{K_{mUDPG\_Suc7}}+\frac{[PPi]_{MC}}{K_{mPPi\_Suc7}}+\\&+\frac{[UTP]_{MC}\cdot[G1P]_{MC}}{K_{mUTP\_Suc2}\;K_{mG1P\_Suc2}}+\frac{[UDPG]_{MC}\cdot[PPi]_{MC}}{K_{mUDPG\_Suc2}\;K_{mPPi\_Suc2}}\end{aligned}$$

$$v_{Suc8} = \frac{V_{m\_Suc8}\left(\cdot [F6P]_{MC} \cdot [UDPG]_{MC} - \frac{[SUCP]_{MC} \cdot [UDP]_{MC}}{k_{e\_Suc8}}\right)}{\left([F6P]_{MC} + K'_{mF6P\_Suc8}\right)\left([UDPG]_{MC} + K'_{mUDPG\_Suc8}\right)}$$

$$K'_{mF6P\_Suc8} = K_{mF6P\_Suc8}\left(\cdot 1 + \frac{[FBP]_{MC}}{K_{iFBP\_Suc8}}\right)$$

$$K'_{mUDPG\_Suc8} = K_{mUDPG\_Suc8}\left(\cdot 1 + \frac{[UDP]_{MC}}{K_{iUDP\_Suc8}}\right)\left(1 + \frac{[SUCP]_{MC}}{K_{iSUCP\_Suc8}}\right)\left(1 + \frac{[SUC]_{MC}}{K_{iSUC\_Suc8}}\right)\left(1 + \frac{[Pi]_{MC}}{K_{iPi\_Suc8}}\right)$$

$$v_{Suc9} = \frac{V_{m\_Suc9}\left(\cdot [SUCP]_{MC} - \frac{[SUC]_{MC} \cdot [Pi]_{MC}}{k_{e\_Suc9}}\right)}{[SUCP]_{MC} + K_{mSUCP\_Suc9} \cdot \left(1 + \frac{[SUC]_{MC}}{K_{mSUC\_Suc9}}\right)}$$

$$v_{Suc10} = V_{m\_Suc10} \cdot \frac{[SUC]_{MC}}{\left([SUC]_{MC} + K_{mSUC\_Suc10}\right)}$$

4.1.6 PGA Sink reaction

$$v_{PGAsink} = V_{m\_PGAsink} \cdot \frac{[PGA]_{MC}}{\left([PGA]_{MC} + K_{mPGA\_PGAsink}\right)}$$

4.1.7 Light reactions

$$J_m = \frac{I_m + J_{\max\_m} - \sqrt{\left(I_m + J_{\max\_m}\right)^2 - 4\theta I_m J_{\max\_m}}}{2\theta}$$

$$J_b = \frac{I_b + J_{\max\_b} - \sqrt{\left(I_b + J_{\max\_b}\right)^2 - 4\theta I_b J_{\max\_b}}}{2\theta}$$

$$I_m = X_m \cdot I \cdot abs(1 - f) \cdot \frac{1}{2}$$

$$J_{\max\_m} = Y_m \cdot J_{\max}$$

$$I_b = X_b \cdot I \cdot abs(1 - f)$$

$$J_{\max\_b} = Y_b \cdot J_{\max}$$

$$v_{ATPM} = \frac{\min(V_{m\_ATPM}, D \cdot J_m) \cdot \left([ADP]_{MC} \cdot [Pi]_{MC} - \frac{[ATP]_{MC}}{k_{e\_ATPM}} \right)}{K_{mADP\_ATPM} \cdot K_{mPi\_ATPM} \cdot \alpha_{ATPM}}$$

$$\alpha_{ATPM} = 1 + \frac{[ADP]_{MC}}{K_{mADP\_ATPM}} + \frac{[Pi]_{MC}}{K_{mPi\_ATPM}} + \frac{[ATP]_{MC}}{K_{mATP\_ATPM}} + \frac{[ADP]_{MC} \cdot [Pi]_{MC}}{K_{mADP\_ATPM} \cdot K_{mPi\_ATPM}}$$

$$v_{NADPHM} = \frac{\min(V_{m\_ATPM}, E \cdot J_m) \cdot \left([NADP]_{MC} - \frac{[NADPH]_{MC}}{k_{e\_NADPM}} \right)}{K_{mNADP\_NADPHM} \cdot \left(1 + \frac{[NADP]_{MC}}{K_{mNADP\_NADPHM}} + \frac{[NADPH]_{MC}}{K_{mNADPH\_NADPHM}} \right)}$$

$$v_{ATPB} = \frac{\min(V_{m\_ATPB}, G \cdot J_b) \cdot \left([ADP]_{BSC} \cdot [Pi]_{BSC} - \frac{[ATP]_{BSC}}{k_{e\_ATPB}} \right)}{K_{mADP\_ATPB} \cdot K_{mPi\_ATPB} \cdot \alpha_{ATPB}}$$

$$\alpha_{ATPB} = 1 + \frac{[ADP]_{BSC}}{K_{mADP\_ATPB}} + \frac{[Pi]_{BSC}}{K_{mPi\_ATPB}} + \frac{[ATP]_{BSC}}{K_{mATP\_ATPB}} + \frac{[ADP]_{BSC} \cdot [Pi]_{BSC}}{K_{mADP\_ATPB} \cdot K_{mPi\_ATPB}}$$

4.1.8 PGA<->PEP reaction

$$v_{Ex} = \frac{V_{m\_Ex} \cdot \left([PGA]_{MC} - \frac{[PEP]_{MC}}{k_{e\_Ex}} \right)}{K_{mPGA\_Ex} \cdot \left(1 + \frac{[PGA]_{MC}}{K_{mPGA\_Ex}} + \frac{[PEP]_{MC}}{K_{mPEP\_Ex}} \right)}$$

4.1.9 Photorespiration reactions

$$v_{\mathrm{Pr1}} = \frac{V'_{m\_\mathrm{Pr1}} \min\left(1, \frac{[RuBP]_{Bchl}}{[Rubisco]_{Bchl}} \right) \cdot [RuBP]_{Bchl} \cdot [O_2]_{Bchl}}{([O_2]_{Bchl} + K'_{mO_2\_\mathrm{Pr1}})([RuBP]_{Bchl} + K'_{mRuBP\_\mathrm{Pr1}})}$$

$$V'_{m\_\mathrm{Pr1}} = V_{m\_\mathrm{Pr1}} \cdot \frac{[CO_2]_{Bchl}}{K_{ACO_2\_\mathrm{Pr1}} + [CO_2]_{Bchl}}$$

$$K'_{mO_2\_\mathrm{Pr1}} = K_{mO_2\_\mathrm{Pr1}} \cdot (1 + \frac{[CO_2]_{Bchl}}{K_{iCO_2\_\mathrm{Pr1}}})$$

$$K'_{mRuBP\_\mathrm{Pr1}} = K_{mRuBP\_\mathrm{Pr1}} \cdot (1 + \frac{[PGA]_{Bchl}}{K_{iPGA\_\mathrm{Pr1}}} + \frac{[FBP]_{Bchl}}{K_{iFBP\_\mathrm{Pr1}}} + \frac{[SBP]_{Bchl}}{K_{iSBP\_\mathrm{Pr1}}} + \frac{[Pi]_{Bchl}}{K_{iPi\_\mathrm{Pr1}}} + \frac{[NADPH]_{Bchl}}{K_{iNADPH\_\mathrm{Pr1}}})$$

$$v_{\mathrm{Pr2}} = \frac{V_{m\_\mathrm{Pr2}} \cdot [PGCA]_{Bchl}}{\left([PGCA]_{Bchl} + K_{mPGCA\_\mathrm{Pr2}} \cdot \left(1 + \frac{[GCA]_{Bchl}}{K_{iGCA\_\mathrm{Pr2}}}\right)\left(1 + \frac{[Pi]_{Bchl}}{K_{iPi\_\mathrm{Pr2}}}\right)\right)}$$

$$v_{\mathrm{Pr3}} = \frac{V_{m\_\mathrm{Pr3}} \cdot [GCA]_{Bper}}{\left([GCA]_{Bper} + K_{mGCA\_\mathrm{Pr3}}\right)}$$

$$v_{\mathrm{Pr4}} = \frac{V_{m\_\mathrm{Pr4}} \cdot \left([GOA]_{Bper} \cdot [GLU]_{Bper} - \frac{[KG]_{Bper} \cdot [GLY]_{Bper}}{k_{e\_\mathrm{Pr4}}}\right)}{\left([GOA]_{Bper} + K_{mGOA\_\mathrm{Pr4}}\right)\left([GLU]_{Bper} + K_{mGLU\_\mathrm{Pr4}} \cdot \left(1 + \frac{[GLY]_{Bper}}{K_{iGLY\_\mathrm{Pr4}}}\right)\right)}$$

$$v_{\mathrm{Pr5}} = \frac{V_{m\_\mathrm{Pr5}} \cdot [GLY]_{Bper}}{[GLY]_{Bper} + K_{mGLY\_\mathrm{Pr5}} \cdot \left(1 + \frac{[SER]_{Bper}}{K_{iSER\_\mathrm{Pr5}}}\right)}$$

$$v_{\mathrm{Pr6}} = \frac{V_{m\_\mathrm{Pr6}} \cdot \left([GOA]_{Bper} \cdot [SER]_{Bper} - \frac{[HPR]_{Bper} \cdot [GLY]_{Bper}}{k_{e\_\mathrm{Pr6}}}\right)}{\left([GOA]_{Bper} + K_{mGOA\_\mathrm{Pr6}}\right)\left([SER]_{Bper} + K_{mSER\_\mathrm{Pr6}} \cdot \left(1 + \frac{[GLY]_{Bper}}{K_{iGLY\_\mathrm{Pr6}}}\right)\right)}$$

$$v_{\mathrm{Pr7}} = \frac{V_{m\_\mathrm{Pr7}} \cdot \left([HPR]_{Bper} \cdot [NADH]_{Bper} - \frac{[NAD]_{Bper} \cdot [GCEA]_{Bper}}{k_{e\_\mathrm{Pr7}}}\right)}{\left([HPR]_{Bper} + K_{mHPR\_\mathrm{Pr6}} \cdot \left(1 + \frac{[HPR]_{Bper}}{K_{iHPR\_\mathrm{Pr7}}}\right)\right)}$$

$$v_{\mathrm{Pr8}} = \frac{V_{m\_\mathrm{Pr8}} \cdot \left([ATP]_{Bchl} \cdot [GCEA]_{Bchl} - \dfrac{[ADP]_{Bchl} \cdot [PGA]_{Bchl}}{k_{e\_\mathrm{Pr8}}} \right)}{\left([GCEA]_{Bchl} + K_{mGCEA\_\mathrm{Pr8}} \right) \left([ATP]_{Bchl} + K_{mATP\_\mathrm{Pr8}} \cdot \left(1 + \dfrac{[PGA]_{Bchl}}{K_{iPGA\_\mathrm{Pr8}}} \right) \right)}$$

$$v_{\mathrm{Pr9}} = \frac{V_{m\_\mathrm{Pr9}} \cdot [GCA]_{Bchl}}{\left([GCA]_{Bchl} + K_{mGCA\_\mathrm{Pr9}} \cdot (1 + \dfrac{[GCEA]_{Bchl}}{K_{iGCEA\_\mathrm{Pr9}}}) \right)} - \\ - \frac{V_{m\_\mathrm{Pr9}} \cdot [GCA]_{Bper}}{\left([GCA]_{Bper} + K_{mGCA\_\mathrm{Pr9}} \cdot (1 + \dfrac{[GCEA]_{Bper}}{K_{iGCEA\_\mathrm{Pr9}}}) \right)}$$

$$v_{\mathrm{Pr10}} = \frac{V_{m\_\mathrm{Pr10}} \cdot [GCEA]_{Bper}}{\left([GCEA]_{Bper} + K_{mGCEA\_\mathrm{Pr10}} \cdot (1 + \dfrac{[GCA]_{Bper}}{K_{iGCA\_\mathrm{Pr10}}}) \right)} - \\ - \frac{V_{m\_\mathrm{Pr10}} \cdot [GCEA]_{Bchl}}{\left([GCEA]_{Bchl} + K_{mGCEA\_\mathrm{Pr10}} \cdot (1 + \dfrac{[GCA]_{Bchl}}{K_{iGCA\_\mathrm{Pr10}}}) \right)}$$

4.1.10 CO2 leakage rate

$$\mathrm{v}_{leak\_Bchl} = J_{CO_2\_Bchl} \cdot \frac{S_{chl}}{S_l} = P_{CO_2\_Bchl} \cdot \frac{S_{chl}}{S_l} \cdot \left([CO_2]_{Bchl} - [CO_2]_{BSC} \right)$$

$$\mathrm{v}_{leak} = J_{CO_2\_PD} \cdot \frac{S_{PD}}{S_l} = \frac{D_{CO_2\_PD}}{l_{PD}} \cdot \frac{S_w \cdot \phi}{S_l} \cdot \left([CO_2]_{BSC} - [CO_2]_{MC} \right)$$

$$S_{PD} = S_w \cdot \varphi$$

4.1.11 Metabolite transport reactions

$$\mathrm{v}_{TMAL} = J_{MAL\_PD} \cdot \frac{S_{PD}}{S_l} = \frac{D_{MAL\_PD}}{l_{PD}} \cdot \frac{S_w \cdot \phi}{S_l} \cdot \left([MAL]_{MC} - [MAL]_{BSC} \right)$$

$$\mathrm{v}_{TPYR} = J_{PYR\_PD} \cdot \frac{S_{PD}}{S_l} = \frac{D_{PYR\_PD}}{l_{PD}} \cdot \frac{S_w \cdot \phi}{S_l} \cdot \left([PYR]_{BSC} - [PYR]_{MC} \right)$$

$$\mathrm{v}_{TPGA} = J_{PGA\_PD} \cdot \frac{S_{PD}}{S_l} = \frac{D_{PGA\_PD}}{l_{PD}} \cdot \frac{S_w \cdot \phi}{S_l} \cdot \left([PGA]_{BSC} - [PGA]_{MC}\right)$$

$$\mathrm{v}_{TGAP} = J_{GAP\_PD} \cdot \frac{S_{PD}}{S_l} = \frac{D_{GAP\_PD}}{l_{PD}} \cdot \frac{S_w \cdot \phi}{S_l} \cdot \left([GAP]_{MC} - [PGA]_{BSC}\right)$$

$$\mathrm{v}_{TDHAP} = J_{DHAP\_PD} \cdot \frac{S_{PD}}{S_l} = \frac{D_{DHAP\_PD}}{l_{PD}} \cdot \frac{S_w \cdot \phi}{S_l} \cdot \left([DHAP]_{MC} - [DHAP]_{BSC}\right)$$

$$v_{TOAA\_M} = V_{m\_OAA\_M} \cdot \frac{\left([OAA]_{MC} - \dfrac{[OAA]_{Mchl}}{K_{i\_OAA\_M}}\right)}{[OAA]_{MC} + K_{m\_OAA\_M} \cdot \left(1 + \dfrac{[malate]_{MC}}{K_{imal\_OAA\_M}}\right)}$$

$$v_{TMAL\_M} = \frac{V_{MAL\_M} \cdot \left([MAL]_{Mchl} \text{-} [MAL]_{MC}\right)}{[MAL]_{Mchl} + K_{mMAL\_MAL\_M} \cdot (1 + \dfrac{[OAA]_{Mchl}}{K_{iOAA\_MAL\_M}})}$$

$$v_{TMAL\_B} = \frac{V_{MAL\_B} \cdot \left([MAL]_{BSC} \text{-} [MAL]_{Bchl}\right)}{[MAL]_{BSC} + K_{mMAL\_MAL\_B}}$$

$$v_{TPYR\_B} = \frac{V_{m\_PYR\_B} \cdot [PYR]_{Bchl}}{\left([PYR]_{Bchl} + K_{m\_PYR\_B}\right)}$$

$$v_{TPYR\_M} = \frac{V_{m\_PYR\_M} \cdot [PYR]_{MC}}{[PYR]_{MC} + K_{m\_PYR\_M}}$$

$$v_{TPEP\_M} = \frac{V_{m\_PEP\_M} \cdot [PEP]_{Mchl}}{[PEP]_{Mchl} + K_{m\_PEP\_M}}$$

$$\begin{aligned}
\mathrm{v}_{TPGA\_B} = {} & \frac{V_{m\_C3P\_B} \cdot [PGA]_{Bchl}}{[PGA]_{Bchl} + K_{mPGA} \cdot \left(1 + \dfrac{[DHAP]_{Bchl}}{K_{mDHAP}}\right)\left(1 + \dfrac{[GAP]_{Bchl}}{K_{mGAP}}\right)} - \\
& - \frac{V_{m\_C3P\_B} \cdot [PGA]_{BSC}}{[PGA]_{BSC} + K_{mPGA} \cdot \left(1 + \dfrac{[DHAP]_{BSC}}{K_{mDHAP}}\right)\left(1 + \dfrac{[GAP]_{BSC}}{K_{mGAP}}\right)}
\end{aligned}$$

$$\mathrm{v}_{TGAP\_B}=\frac{V_{m\_C3P\_B}\cdot[GAP]_{BSC}}{[GAP]_{BSC}+K_{mGAP}\cdot\left(1+\frac{[DHAP]_{BSC}}{K_{mDHAP}}\right)\left(1+\frac{[PGA]_{BSC}}{K_{mPGA}}\right)}-$$

$$-\frac{V_{m\_C3P\_B}\cdot[GAP]_{Bchl}}{[GAP]_{Bchl}+K_{mGAP}\cdot\left(1+\frac{[DHAP]_{Bchl}}{K_{mDHAP}}\right)\left(1+\frac{[PGA]_{Bchl}}{K_{mPGA}}\right)}$$

$$\mathrm{v}_{TDHAP\_B}=\frac{V_{m\_C3P\_B}\cdot[DHAP]_{BSC}}{[DHAP]_{BSC}+K_{mDHAP}\cdot\left(1+\frac{[GAP]_{BSC}}{K_{mGAP}}\right)\left(1+\frac{[PGA]_{BSC}}{K_{mPGA}}\right)}-$$

$$-\frac{V_{m\_C3P\_B}\cdot[DHAP]_{Bchl}}{[DHAP]_{Bchl}+K_{mDHAP}\cdot\left(1+\frac{[GAP]_{Bchl}}{K_{mGAP}}\right)\left(1+\frac{[PGA]_{Bchl}}{K_{mPGA}}\right)}$$

$$\mathrm{v}_{TPGA\_M}=\frac{V_{m\_C3P\_B}\cdot[PGA]_{MC}}{[PGA]_{MC}+K_{mPGA}\cdot\left(1+\frac{[DHAP]_{MC}}{K_{mDHAP}}\right)\left(1+\frac{[GAP]_{MC}}{K_{mGAP}}\right)}-$$

$$-\frac{V_{m\_C3P\_B}\cdot[PGA]_{Mchl}}{[PGA]_{Mchl}+K_{mPGA}\cdot\left(1+\frac{[DHAP]_{Mchl}}{K_{mDHAP}}\right)\left(1+\frac{[GAP]_{Mchl}}{K_{mGAP}}\right)}$$

$$\mathrm{v}_{TGAP\_M}=\frac{V_{m\_C3P\_B}\cdot[GAP]_{Mchl}}{[GAP]_{Mchl}+K_{mGAP}\cdot\left(1+\frac{[DHAP]_{Mchl}}{K_{mDHAP}}\right)\left(1+\frac{[PGA]_{Mchl}}{K_{mPGA}}\right)}-$$

$$-\frac{V_{m\_C3P\_B}\cdot[GAP]_{MC}}{[GAP]_{MC}+K_{mGAP}\cdot\left(1+\frac{[DHAP]_{MC}}{K_{mDHAP}}\right)\left(1+\frac{[PGA]_{MC}}{K_{mPGA}}\right)}$$

$$\mathrm{v}_{TDHAP\_M}=\frac{V_{m\_C3P\_B}\cdot[DHAP]_{Mchl}}{[DHAP]_{Mchl}+K_{mDHAP}\cdot\left(1+\frac{[GAP]_{Mchl}}{K_{mGAP}}\right)\left(1+\frac{[PGA]_{Mchl}}{K_{mPGA}}\right)}-$$

$$-\frac{V_{m\_C3P\_B}\cdot[DHAP]_{MC}}{[DHAP]_{MC}+K_{mDHAP}\cdot\left(1+\frac{[GAP]_{MC}}{K_{mGAP}}\right)\left(1+\frac{[PGA]_{MC}}{K_{mPGA}}\right)}$$

4.1.12 Carbon isotope (13CO2) discrimination

$$^{13}C_i = C_i \cdot R_a \cdot \frac{1}{\alpha_0}$$

$$^{12}C_i = C_i \cdot (1 - R_a \cdot \frac{1}{\alpha_0})$$

$$v_{inf\_h} = g_m \cdot \frac{1}{S_c} \cdot 10^{-3} \frac{1}{\alpha_1} \cdot (^{13}C_i - [^{13}CO_2]_{MC})$$

$$v'_{inf} = g_m \cdot \frac{1}{S_c} \cdot 10^{-3} (^{12}C_i - [^{12}CO_2]_{MC})$$

$$v_{1\_h} = v_1 \cdot \frac{1}{\alpha_2} \cdot \frac{1}{\alpha_3} \cdot \frac{[^{13}CO_2]_{MC}}{[^{12}CO_2]_{MC}}$$

$$v_{2\_h} = v_2 \cdot \frac{1}{\alpha_4} \cdot \frac{[H^{13}CO_3]_{Bchl}}{[H^{12}CO_3]_{Bchl}}$$

$$v_{4\_h} = v_4 \cdot \frac{v_{2\_h}}{v_2}$$

$$v_{6\_h} = v_6 \cdot \frac{1}{\alpha_5} \cdot \frac{[^{13}CO_2]_{Bchl}}{[^{12}CO_2]_{Bchl}}$$

$$\mathrm{v}_{leak\_Bchl\_h} = P_{CO_2\_Bchl} \cdot \frac{S_{chl}}{S_l} \cdot \frac{1}{\alpha_6} \cdot \left([^{13}CO_2]_{Bchl} - [^{13}CO_2]_{BSC}\right)$$

$$v_{leak\_h} = \frac{D_{CO_2\_PD}}{l_{PD}} \cdot \frac{S_w \cdot \varphi}{S_l} \cdot \frac{1}{\alpha_6} \left([^{13}CO_2]_{BSC} - [^{13}CO_2]_{MC}\right)$$

$$R_{d\_h} = R_d \cdot \frac{R_a}{1 + \Delta_l}$$

$$R'_d = R_d \cdot (1 - \frac{R_a}{1 + \Delta_l})$$

$$v_{pr5\_h} = v_{pr5} \cdot \frac{R_a}{1 + \Delta_l}$$

$$v'_{pr5} = v_{pr5} \cdot (1 - \frac{R_a}{1 + \Delta_l})$$

4.2. Differential Equations

4.2.1. Metabolite concentration changes in mesophyll cell cytosol

$$\frac{d[CO_2]_{MC}}{dt} = \left(v_{\inf} - v_1 + v_{leak} + R_m\right) \cdot \frac{1}{Vol_{Mcyto}}$$

$$\frac{d[HCO_3]_{MC}}{dt} = \left(v_1 - v_2\right) \cdot \frac{1}{Vol_{Mcyto}}$$

$$\frac{d[OAA]_{MC}}{dt} = \left(v_2 - v_{OAA\_M}\right) \cdot \frac{1}{Vol_{Mcyto}}$$

$$\frac{d[PEP]_{MC}}{dt} = \left(v_{PEP\_M} - v_2 + v_{Ex}\right) \cdot \frac{1}{Vol_{Mcyto}}$$

$$\frac{d[Malate]_{MC}}{dt} = \left(v_{MAL\_M} - v_{MAL}\right) \cdot \frac{1}{Vol_{Mcyto}}$$

$$\frac{d[Pyruvate]_{MC}}{dt} = \left(v_{PYR} - v_{PYR\_M}\right) \cdot \frac{1}{Vol_{Mcyto}}$$

$$\frac{d[PGA]_{MC}}{dt} = \left(v_{PGA} - v_{PGA\_M} - v_{Ex} - v_{PGASink}\right) \cdot \frac{1}{Vol_{Mcyto}}$$

$$\frac{d[FBP]_{MC}}{dt} = \left(v_{Suc1} - v_{Suc2}\right) \cdot \frac{1}{Vol_{Mcyto}}$$

$$\frac{d[UDPG]_{MC}}{dt} = \left(v_{Suc7} - v_{Suc8}\right) \cdot \frac{1}{Vol_{Mcyto}}$$

$$\frac{d[SUCP]_{MC}}{dt} = \left(v_{Suc8} - v_{Suc9}\right) \cdot \frac{1}{Vol_{Mcyto}}$$

$$\frac{d[SUC]_{MC}}{dt} = \left(v_{Suc9} - v_{Suc10}\right) \cdot \frac{1}{Vol_{Mcyto}}$$

$$\frac{d[F26BP]_{MC}}{dt} = \left(v_{Suc3} - v_{Suc4}\right) \cdot \frac{1}{Vol_{Mcyto}}$$

$$\frac{d[ATP]_{MC}}{dt} = \left(v_{tATP\_M} - v_{Suc7} - v_{Suc3}\right) \cdot \frac{1}{Vol_{Mcyto}}$$

$$\frac{d[T3P]_{MC}}{dt} = \left(v_{GAP\_M} + v_{DHAP\_M} - v_{GAP} - v_{DHAP} - 2v_{Suc1}\right) \cdot \frac{1}{Vol_{Mcyto}}$$

$$\frac{d[HexP]_{MC}}{dt} = \left(v_{Suc2} + v_{Suc4} - v_{Suc3} - v_{Suc7} - v_{Suc8}\right) \cdot \frac{1}{Vol_{Mcyto}}$$

4.2.2. Metabolite concentration changes in mesophyll cell chloroplast

$$\frac{d[OAA]_{Mchl}}{dt} = \left(v_{OAA\_M} - v_3\right) \cdot \frac{1}{Vol_{Mchl}}$$

$$\frac{d[Malate]_{Mchl}}{dt} = \left(v_3 - v_{MAL\_M}\right) \cdot \frac{1}{Vol_{Mchl}}$$

$$\frac{d[PEP]_{Mchl}}{dt} = \left(v_5 - v_{PEP\_M}\right) \cdot \frac{1}{Vol_{Mchl}}$$

$$\frac{d[Pyruvate]_{Mchl}}{dt} = \left(v_{PYR\_M} - v_5\right) \cdot \frac{1}{Vol_{Mchl}}$$

$$\frac{d[NADPH]_{Mchl}}{dt} = \left(v_{NADGPHM} - v_3 - v_{8Mchl}\right) \cdot \frac{1}{Vol_{Mchl}}$$

$$\frac{d[ATP]_{Mchl}}{dt} = \left(v_{ATPM} - 2v_5 - v_{7Mchl} - v_{tATP}\right) \cdot \frac{1}{Vol_{Mchl}}$$

$$\frac{d[PGA]_{Mchl}}{dt} = \left(v_{PGA\_M} - v_{7Mchl}\right) \cdot \frac{1}{Vol_{Mchl}}$$

$$\frac{d[T3P]_{Mchl}}{dt} = \left(v_{8Mchl} - v_{GAP\_M} - v_{DHAP\_M}\right) \cdot \frac{1}{Vol_{Mchl}}$$

4.2.3. Metabolite concentration changes in bundle sheath cell cytosol

$$\frac{d[T3P]_{BSC}}{dt} = \left(v_{GAP} + v_{DHAP} - v_{GAP\_B} - v_{DHAP\_B}\right) \cdot \frac{1}{Vol_{Bcyto}}$$

$$\frac{d[PGA]_{BSC}}{dt} = \left(v_{PGA\_B} - v_{PGA}\right) \cdot \frac{1}{Vol_{Bcyto}}$$

$$\frac{d[Malate]_{BSC}}{dt} = \left(v_{MAL} - v_{MAL\_B}\right) \cdot \frac{1}{Vol_{Bcyto}}$$

$$\frac{d[Pyruvate]_{BSC}}{dt} = \left(v_{PYR\_B} - v_{PYR}\right) \cdot \frac{1}{Vol_{Bcyto}}$$

$$\frac{d[CO_2]_{BSC}}{dt} = \left(v_{leak\_Bchl} + v_{\mathrm{Pr}5} + R_b - v_{leak}\right) \cdot \frac{1}{Vol_{Bcyto}}$$

4.2.4. Metabolite concentration changes in bundle sheath cell chloroplast

$$\frac{d[CO_2]_{Bchl}}{dt}=\left(v_4-v_6-v_{leak\_Bchl}\right)\cdot\frac{1}{Vol_{Bchl}}$$

$$\frac{d[RuBP]_{Bchl}}{dt}=\left(v_{18}-v_6-v_{Pr1}\right)\cdot\frac{1}{Vol_{Bchl}}$$

$$\frac{d[PGA]_{Bchl}}{dt}=\left(2v_6-v_7-v_{PGA\_B}+v_{Pr1}+v_{Pr8}\right)\cdot\frac{1}{Vol_{Bchl}}$$

$$\frac{d[ATP]_{Bchl}}{dt}=\left(v_{ATPB}-v_7-v_{18}-v_{sta3}-v_{Pr8}\right)\cdot\frac{1}{Vol_{Bchl}}$$

$$\frac{d[NADPH]_{Bchl}}{dt}=\left(v_4-v_8\right)\cdot\frac{1}{Vol_{Bchl}}$$

$$\frac{d[SBP]_{Bchl}}{dt}=\left(v_{12}-v_{13}\right)\cdot\frac{1}{Vol_{Bchl}}$$

$$\frac{d[S7P]_{Bchl}}{dt}=\left(v_{13}-v_{15}\right)\cdot\frac{1}{Vol_{Bchl}}$$

$$\frac{d[FBP]_{Bchl}}{dt}=\left(v_{10}-v_{11}\right)\cdot\frac{1}{Vol_{Bchl}}$$

$$\frac{d[E4P]_{Bchl}}{dt}=\left(v_{14}-v_{12}\right)\cdot\frac{1}{Vol_{Bchl}}$$

$$\frac{d[T3P]_{Bchl}}{dt}=\left(v_{GAP\_B}+v_{DHAP\_B}+v_8-2v_{10}-v_{14}-v_{15}-v_{12}\right)\cdot\frac{1}{Vol_{Bchl}}$$

$$\frac{d[HexP]_{Bchl}}{dt}=\left(v_{11}-v_{14}-v_{Sta3}\right)\cdot\frac{1}{Vol_{Bchl}}$$

$$\frac{d[Pent]_{Bchl}}{dt}=\left(v_{14}+2v_{15}-v_{18}\right)\cdot\frac{1}{Vol_{Bchl}}$$

$$\frac{d[Malate]_{Bchl}}{dt}=\left(v_{MAL\_B}-v_4\right)\cdot\frac{1}{Vol_{Bchl}}$$

$$\frac{d[Pyruvate]_{Bchl}}{dt}=\left(v_4-v_{PYR\_B}\right)\cdot\frac{1}{Vol_{Bchl}}$$

$$\frac{d[PPi]_{Bchl}}{dt}=\left(v_{Sta3}-v_{Sta4}\right)\cdot\frac{1}{Vol_{Bchl}}$$

$$\frac{d[ADPG]_{Bchl}}{dt} = \left(v_{Sta3} - v_{Sta5}\right) \cdot \frac{1}{Vol_{Bchl}}$$

$$\frac{d[PGCA]_{Bchl}}{dt} = \left(v_{Pr1} - v_{Pr2}\right) \cdot \frac{1}{Vol_{Bchl}}$$

$$\frac{d[GCA]_{Bchl}}{dt} = \left(v_{Pr2} - v_{Pr9}\right) \cdot \frac{1}{Vol_{Bchl}}$$

$$\frac{d[GCEA]_{Bchl}}{dt} = \left(v_{Pr10} - v_{Pr8}\right) \cdot \frac{1}{Vol_{Bchl}}$$

4.2.5. Metabolite concentration changes in bundle sheath cell peroxisome

$$\frac{d[GCA]_{Bper}}{dt} = \left(v_{Pr9} - v_{Pr3}\right) \cdot \frac{1}{Vol_{Bper}}$$

$$\frac{d[GOA]_{Bper}}{dt} = \left(v_{Pr3} - v_{Pr4} - v_{Pr6}\right) \cdot \frac{1}{Vol_{Bper}}$$

$$\frac{d[GLY]_{Bper}}{dt} = \left(v_{Pr4} + v_{Pr6} - 2v_{Pr5}\right) \cdot \frac{1}{Vol_{Bper}}$$

$$\frac{d[SER]_{Bper}}{dt} = \left(v_{Pr5} - v_{Pr6}\right) \cdot \frac{1}{Vol_{Bper}}$$

$$\frac{d[HPR]_{Bper}}{dt} = \left(v_{Pr6} - v_{Pr7}\right) \cdot \frac{1}{Vol_{Bper}}$$

$$\frac{d[GCEA]_{Bper}}{dt} = \left(v_{Pr7} - v_{Pr10}\right) \cdot \frac{1}{Vol_{Bper}}$$

4.2.6. Metabolite concentration changes for calculation of Carbon isotope ($^{13}CO_2$) discrimination

$$\frac{d[CO_2]'_{MC}}{dt} = \left(v'_{\inf} - v_1 + v_{leak} + R'_m\right) \cdot \frac{1}{Vol_{Mcyto}}$$

$$\frac{d[OAA]'_{MC}}{dt} = \left((v_2 + v_{2\_h}) - v_{OAA\_M}\right) \cdot \frac{1}{Vol_{Mcyto}}$$

$$\frac{d[PEP]'_{MC}}{dt} = \left(v_{PEP\_M} - (v_2 + v_{2\_h}) + v_{Ex}\right) \cdot \frac{1}{Vol_{Mcyto}}$$

$$\frac{d[CO_2]'_{BSC}}{dt} = \left(v_{leak\_Bchl} + v'_{\mathrm{Pr}5} + R'_b - v_{leak}\right) \cdot \frac{1}{Vol_{Bcyto}}$$

$$\frac{d[RuBP]'_{Bchl}}{dt} = \left(v_{18} - (v_6 + v_{6\_h}) - v_{Pr1}\right) \cdot \frac{1}{Vol_{Bchl}}$$

$$\frac{d[PGA]'_{Bchl}}{dt} = \left(2 \cdot (v_6 + v_{6\_h}) - v_7 - v_{PGA\_B} + v_{Pr1} + v_{Pr8}\right) \cdot \frac{1}{Vol_{Bchl}}$$

$$\frac{d[Malate]'_{Bchl}}{dt} = \left(v_{MAL\_B} - (v_4 + v_{4\_h})\right) \cdot \frac{1}{Vol_{Bchl}}$$

$$\frac{d[Pyruvate]'_{Bchl}}{dt} = \left((v_4 + v_{4\_h}) - v_{PYR\_B}\right) \cdot \frac{1}{Vol_{Bchl}}$$

$$\frac{d[NADPH]'_{Bchl}}{dt} = \left((v_4 + v_{4\_h}) - v_8\right) \cdot \frac{1}{Vol_{Bchl}}$$

$$\frac{d[^{13}CO_2]_{MC}}{dt} = \left(v_{\inf\_h} - v_{1\_h} + v_{leak\_h} + R'_{m\_h}\right) \cdot \frac{1}{Vol_{Mcyto}}$$

$$\frac{d[H^{13}CO_3]_{MC}}{dt} = \left(v_{1\_h} - v_{2\_h}\right) \cdot \frac{1}{Vol_{Mcyto}}$$

$$\frac{d[^{13}CO_2]_{BSC}}{dt} = \left(v_{leak\_Bchl\_h} + v_{\mathrm{Pr}5\_h} + R_{b\_h} - v_{leak\_h}\right) \cdot \frac{1}{Vol_{Bcyto}}$$

$$\frac{d[^{13}CO_2]_{Bchl}}{dt} = \left(v_{4\_h} - v_{6\_h} - v_{leak\_Bchl\_h}\right) \cdot \frac{1}{Vol_{Bchl}}$$

4.3. Constants

4.3.1. Constants in mesophyll cell cytosol

$$[CA]_{MC} = [ATP]_{MC} - [ADP]_{MC}$$

$$[CU]_{MC} = [UDP]_{MC} + [UTP]_{MC} + [UDPG]_{MC}$$

$$\begin{aligned}[CP]_{MC} = {} & [PiT]_{MC} + 2[FBP]_{MC} + 2[F26BP]_{MC} + [PGA]_{MC} + [T3P]_{MC} + \\ & + [HexP]_{MC} + [SUCP]_{MC} + [UTP]_{MC} + [ATP]_{MC} + [PEP]_{MC}\end{aligned}$$

$$[Pi]_{MC} = \frac{1}{2}(\sqrt{K_{ePi}{}^2 + 4 \cdot K_{ePi} \cdot [PiT]_{MC}} - K_{ePi})$$

$$[PPi]_{MC} = [PiT]_{MC} - [Pi]_{MC}$$

$$[GAP]_{MC} = \frac{K_{e\_9} \cdot [T3P]_{MC}}{(1 + K_{e\_9})}$$

$$[DHAP]_{MC} = \frac{[T3P]_{MC}}{(1 + K_{e\_9})}$$

$$[G6P]_{MC} = \frac{[HexP]_{MC}}{\frac{1}{K_{e\_Suc5}} + K_{e\_Suc6} + 1}$$

$$[G1P]_{MC} = \frac{K_{e\_Suc6} \cdot [HexP]_{MC}}{\frac{1}{K_{e\_Suc5}} + K_{e\_Suc6} + 1}$$

$$[F6P]_{MC} = \frac{\frac{[HexP]_{MC}}{K_{e\_Suc5}}}{\frac{1}{K_{e\_Suc5}} + K_{e\_Suc6} + 1}$$

4.3.2. Constants in mesophyll cell chloroplast

$$[CA]_{Mchl} = [ATP]_{Mchl} + [ADP]_{Mchl}$$

$$[CN]_{Mchl} = [NADPH]_{Mchl} + [NADP]_{Mchl}$$

$$[CP]_{Mchl} = [Pi]_{Mchl} + [PGA]_{Mchl} + 2[DPGA]_{Mchl} + [T3P]_{Mchl} + [ATP]_{Mchl} + [PEP]_{Mchl}$$

$$[GAP]_{Mchl} = \frac{K_{e\_9} \cdot [T3P]_{Mchl}}{(1 + K_{e\_9})}$$

$$[DHAP]_{Mchl} = \frac{[T3P]_{Mchl}}{(1 + K_{e\_9})}$$

4.3.3. Conatants in bundle sheath cell cytosol

$$[GAP]_{BSC} = \frac{K_{e\_9} \cdot [T3P]_{BSC}}{(1 + K_{e\_9})}$$

$$[DHAP]_{BSC} = \frac{[T3P]_{BSC}}{(1 + K_{e\_9})}$$

4.3.4. Conatants in bundle sheath cell chloroplast

$$[CA]_{Bchl} = [ATP]_{Bchl} + [ADP]_{Bchl} + [ADPG]_{Bchl}$$

$$[CN]_{Bchl} = [NADPH]_{Bchl} + [NADP]_{Bchl}$$

$$\begin{aligned}[CP]_{Bchl} = {} & [Pi]_{Bchl} + [PGA]_{Bchl} + 2[DPGA]_{Bchl} + [T3P]_{Bchl} + 2[FBP]_{Bchl} + \\ & + [HexP]_{Bchl} + [E4P]_{Bchl} + 2[SBP]_{Bchl} + [S7P]_{Bchl} + [Pent]_{Bchl} + \\ & + 2[RuBP]_{Bchl} + [ATP]_{Bchl} + [PGCA]_{Bchl} + 2[PPi]_{Bchl}\end{aligned}$$

$$[GAP]_{Bchl} = \frac{K_{e\_9} \cdot [T3P]_{Bchl}}{(1 + K_{e\_9})}$$

$$[DHAP]_{Bchl} = \frac{[T3P]_{Bchl}}{(1 + K_{e\_9})}$$

$$[G6P]_{Bchl} = \frac{[HexP]_{Bchl}}{\frac{1}{K_{e\_Sta1}} + K_{e\_Sta2} + 1}$$

$$[G1P]_{Bchl} = \frac{K_{e\_Sta2} \cdot [HexP]_{Bchl}}{\frac{1}{K_{e\_Sta1}} + K_{e\_Sta2} + 1}$$

$$[F6P]_{Bchl} = \frac{\frac{[HexP]_{Bchl}}{K_{e\_Sta1}}}{\frac{1}{K_{e\_Sta1}} + K_{e\_Sta2} + 1}$$

$$[Xu5P]_{Bchl} = \frac{\frac{[PenP]_{Bchl}}{K_{e\_17}}}{\frac{1}{K_{e\_16}} + \frac{1}{K_{e\_17}} + 1}$$

$$[Ru5P]_{Bchl} = \frac{[PenP]_{Bchl}}{\frac{1}{K_{e\_16}} + \frac{1}{K_{e\_17}} + 1}$$

$$[Ri5P]_{Bchl} = \frac{\frac{[PenP]_{Bchl}}{K_{e\_16}}}{\frac{1}{K_{e\_16}} + \frac{1}{K_{e\_17}} + 1}$$

5 Parameters

5.1 Vmax of photosynthetic enzymes

EC	Numbering	Vmax (μmol m-2 s-1)	Reference
4.2.1.1	1	200000 or variable	Hatch and Burnell (1990) with modification
4.1.1.31	2	170 or variable	Kanai and Edwards (1999), Hatch (1987), von Caemmerer (2000) with modification
1.1.1.82	3	90 or variable	Kanai and Edwards (1999), Hatch (1987) with modification
1.1.1.40	4	90 or variable	Kanai and Edwards (1999), Hatch (1987) with modification
2.7.9.1	5	90 or variable	Kanai and Edwards (1999), Hatch (1987) with modification
4.1.1.39	6	65 or variable	Kanai and Edwards (1999), Hatch (1987), von Caemmerer (2000) with modification
2.7.2.3 & 1.2.1.13	7 and 8	225 or variable	Laisk and Edwards. (2000), with modification
4.1.2.13FBP	10	58.5 or variable	Zhu *et al.* (2007) with modification
3.1.3.11	11	43.6 or variable	Zhu *et al.* (2007) with modification
4.1.2.13SBP	12	110 or variable	Zhu *et al.* (2007) with modification
3.1.3.37	13	29.2 or variable	Zhu *et al.* (2007) with modification
2.2.1.1X	14	281 or variable	Zhu *et al.* (2007) with modification
2.2.1.1R	15	281 or variable	Zhu *et al.* (2007) with modification
2.7.1.19	18	1170 or variable	Zhu *et al.* (2007) with modification
2.7.2.3M & 1.2.1.13M	7M and 8M	300 or variable	Laisk and Edwards. (2000), with modification
4.1.2.13FBP	Suc1	8.05 or variable	Zhu *et al.* (2007) with modification

M			
3.1.3.11M	Suc2	6.40 or variable	Zhu *et al.* (2007) with modification
2.7.7.9	Suc7	5.77 or variable	Zhu *et al.* (2007) with modification
2.4.1.14	Suc8	27.8 or variable	Zhu *et al.* (2007) with modification
3.1.3.24	Suc9	27.8 or variable	Zhu *et al.* (2007) with modification
2.7.1.105	Suc3	1.01 or variable	Zhu *et al.* (2007) with modification
3.1.3.46	Suc4	0.841 or variable	Zhu *et al.* (2007) with modification
2.7.7.27	Sta3	30 or variable	Zhu *et al.* (2007) with modification
3.6.1.1	Sta4	1000 or variable	Zhu *et al.* (2007) with modification
2.4.1.21	Sta5	25 or variable	Zhu *et al.* (2007) with modification
StarchDag	StarchDag	0 or 3.6	Assumed
PGASink	PGASink	2 or variable	Zhu *et al.* (2007) with modification
4.1.1.39PR	Pr1	Vm_6*0.11 or variable	Cousins *et al.* (2010) with modification
3.1.3.18	Pr2	2621 or variable	Zhu *et al.* (2007) with modification
1.1.3.15	Pr3	72.8 or variable	Zhu *et al.* (2007) with modification
2.6.1.4	Pr4	137 or variable	Zhu *et al.* (2007) with modification
Gly_ser	Pr5	125 or variable	Zhu *et al.* (2007) with modification
2.6.1.45	Pr6	165 or variable	Zhu *et al.* (2007) with modification
1.1.1.29	Pr7	500 or variable	Zhu *et al.* (2007) with modification
2.7.1.31	Pr8	286 or variable	Zhu *et al.* (2007) with modification
Tgca	Pr9	300 or variable	Zhu *et al.* (2007) with modification
Tgcea	Pr10	250 or variable	Zhu *et al.* (2007) with modification
5.4.2.1&4.2.1.11	Ex	1 or variable	Laisk and Edwards. (2000), with modification
JmaxM	JmaxM	300 or variable	von Caemmerer (2000) with modification
JmaxB	JmaxB	JmaxM *(1-Y)/Y or variable	Assumed, von Caemmerer (2000) with modification
3.6.3.14M	ATPM	300 or variable	Assumed
3.6.3.14B	ATPB	300 or variable	Assumed

1.18.1.2M	NADPHM	200 or variable	Assumed
TPTM	TPGAM, TDHAPM, TGAPM	750 or variable	Assumed
TPTB	TPGAM, TDHAPM, TGAPM	750 or variable	Assumed
DiT	TOAAM	80 or variable	Assumed
	TmalB	150 or variable	Assumed
	TmalM	150 or variable	Assumed
PPT	TPEPM	150 or variable	Assumed
MEPM	TpyrM	150 or variable	Assumed
MEPB	TpyrB	150 or variable	Assumed

5.2 Michaelis-constant and other paremeters

EC	**Numbering**	**parameters**	**Reference**
	inf	g_m=0.7 mol m^{-2} bar^{-1}	Assumed
		Sc= 0.33 $\times 10^{-4}$ mmol $L^{-1}\mu bar^{-1}$	Uchida *et al.* (1983), Hoofd *et al.* (1986)
4.2.1.1	1	K_{mCO2_1}=2.8 mM	Hatch and Burnell (1990)
		K_{mHCO3_1}=34 mM	Pocker and Miksch (1978)
		[H+]=10e-7.3mM	Felle and Bertl (1986)
		K_{e_1} = 5.6e-7mM	Pocker and Miksch (1978)
4.1.1.31	2	K_{mHCO3_2} =0.02 mM	Uedan and Sugiyama (1976)
		K_{mPEP_2} = 0.1 mM	Mukerji (1977)
		K_{imal_2} =0. 5 mM	Gao and Woo (1996)
1.1.1.82	3	K_{mNADPH_3} =0.024 mM	Kagawa and Bruno (1988)
		K_{mOAA_3} =0.056 mM	Kagawa and Bruno (1988)
		K_{mNADP_3} =0.073 mM	Kagawa and Bruno (1988)
		K_{mmal_3} =32.0 mM	Kagawa and Bruno (1988)
		K_{e_3} =4450.0	Laisk and Edwards (2000)

1.1.1.40	4	K_{mCO2_4} =1.1 mM	Jenkins *et al.* (1987)
		K_{mNADP_4} =0.0080 mM	Detarsio *et al.* (2003)
		K_{mNADPH_4} =0.045 mM	Ziegler (1974)
		K_{mPyr_4} =3.0 mM	Ziegler (1974)
		K_{mmal_4} =0.23 mM	Detarsio *et al.* (2003)
		K_{e_4} =0.051 mM	Harary *et al.* (1953)
2.7.9.1	5	K_{iPEP_5} =0.15 mM	Jenkins and Hatch (1985)
		K_{mATP_5} =0.082 mM	Jenkins and Hatch (1985)
		K_{mPyr_5} =0.082 mM	Jenkins and Hatch (1985)
4.1.1.39	6	K_{mCO2_6} =0.0162 mM	Cousins *et al.* (2010)
		K_{mO2_6} =0.222 mM	Cousins *et al.* (2010)
		K_{mRuBP_6} =0.02 mM	Farquhar (1979)
		K_{iPGA_6} =2.52 mM	Assumed, Badger and Lorimer (1981)
		K_{iFBP_6} =0.04 mM	Badger and Lorimer (1981)
		K_{iSBP_6} =0.75 mM	Badger and Lorimer (1981)
		K_{iPi_6} =3.6 mM	Assumed, Badger and Lorimer (1981)
		K_{iNADPH_6} =0.21 mM	Assumed, Badger and Lorimer (1981)
2.7.2.3 & 1.2.1.13	7 and 8	K_{mPGA_78}=1 mM	Laisk and Edwards (2000)
		K_{mATP_78}=0.3 mM	Laisk and Edwards (2000)
		K_{mNADPH_78}=0.05 mM	Ferri *et al.*(1978), Trost (1993), Macioszek and Anderson (1987), Baalmann *et al.*, 1995, Sparla *et al.*, (2004), Sparla *et al.*, (2005),
5.3.1.1	9	K_{e_9}=0.05	Bassham and Krause (1969)

4.1.2.13FBP	10	K_{mDHAP_10} =0.4 mM	Iwaki *et al.* (1991)
		K_{mGAP_10} =0.3 mM	Iwaki *et al.* (1991), Zhu *et al.* (2007)
		K_{mFBP_10} =0.02 mM	Brooks and Criddle (1966), Schnarrenberger and Kruger (1986)
		K_{e_10} =7.1 mM^{-1}	Bassham and Krause (1969), Iwaki *et al.* (1991)
3.1.3.11	11	K_{iF6P_11} =0.7 mM	Heldt (1983)
		K_{iPi_11} =12.0 mM	Charles and Halliwell (1981)
		K_{mFBP_11} =0.033 mM	Charles and Halliwell (1981)
		K_{e_11} =666000.0 mM	Bassham and Krause (1969) , Laisk *et al.*(1989)
4.1.2.13SBP	12	K_{mDHAP_12} =0.4 mM	Iwaki *et al.* (1991)
		K_{mE4P_12} =0.2 mM	Zhu *et al.* (2007)
		K_{mSBP_12}=0.02 mM	Brooks and Criddle (1966)
		K_{e_12} =1.017 mM^{-1}	Bassham and Krause (1969) , Laisk *et al.*(1989)
3.1.3.37	13	K_{iPi_13} =12.0 mM	Woodrow *et al.* (1983)
		K_{mSBP_13} =0.05 mM	Woodrow *et al.* (1983), Cadet and Meunier (1988)
		K_{e_13} =666000.0 mM	Bassham and Krause (1969), Laisk *et al.*(1989)
2.2.1.1X	14	K_{mE4P_14} =0.1 mM	Zhu *et al.* (2007)
		K_{mF6P_14} =0.1 mM	Zhu *et al.* (2007)
		K_{mGAP_14} =0.1 mM	Sprenger *et al.* (1995), Schenk *et al.*

			(1998), Zhu *et al*. (2007)
		K_{mXu5P} =0.1 mM	Schenk *et al.* (1998), Laisk *et al.* (1989), Zhu *et al*. (2007)
		K_{e_14} =0.084	Datta *et al*. (1961).
2.2.1.1R	15	K_{mGAP_15} =0.072 mM	Albe (1991); Laisk *et al.* (1989)
		K_{mRi5P_15} =1.5 mM	Albe (1991); Laisk *et al.* (1989)
		K_{mS7P_15} =0.46 mM	Albe (1991); Laisk *et al.* (1989)
		K_{mXu5P_15} =0.1 mM	Albe (1991); Laisk *et al.* (1989)
		K_{e_15} =1.176	Bassham and Krause (1969), Laisk *et al.* (1989)
5.3.1.6	16	K_{e_16}=0.4	Bassham and Krause (1969)
5.1.3.1	17	K_{e_17}=0.67	Bassham and Krause, (1969)
2.7.1.19	18	K_{iADP_18} =2.5 mM	Gardemann *et al.* (1983)
		$K_{i\_ADP\_18}$ =0.4 mM	Gardemann *et al.* (1983)
		K_{iPGA_18} =2.0 mM	Gardemann *et al.* (1983)
		K_{iPi_18} =4.0 mM	Gardemann *et al.* (1983)
		K_{iRuBP_18} =0.7 mM	Gardemann *et al.* (1983)
		K_{mATP_18} =0.625 mM	Slabas *et al.* (1976)
		K_{mRu5P_18} =0.05 mM	Gardemann *et al.* (1983), Omnaas *et al.*(1985)
		K_{e_18} =6846.0	Bassham and Krause (1969), Laisk *et al.* (1989)
4.1.2.13FBPM	Suc1	K_{mDHAP_Suc1}=0.45 mM	Iwaki *et al.* (1991)
		K_{mGAP_Suc1} =0.04 mM	Iwaki *et al.* (1991)
		K_{mFBP_Suc1}=0.023 mM	Schnarrenberger (1986)
		K_{e_Suc1} =12.0 mM^{-1}	Thomas *et al.* (1997), Zhu *et al.* (2007)

3.1.3.11M	Suc2	K_{iF26BP_Suc2} =0.007mM	Jang *et al.* (2003)
		K_{iF6P_Suc2} =0.7 mM	Heldt *et al.* (1983)
		K_{iPi_Suc2} =12.0 mM	Charles & Halliwell (1981)
		K_{mFBP_Suc2} =0.0025mM	Jang *et al.* (2003)
		K_{e_Suc2} =174.0 mM	Lawson *et al.* (1976)
5.3.1.9M	Suc5	K_{e_Suc5}=2.3	Bassham and Krause (1969),
5.4.2.2M	Suc6	K_{e_Suc6}=0.0584	Bassham and Krause (1969),
2.7.7.9	Suc7	K_{mG1P_Suc7} =0.14 mM	Nakano *et al.* (1989)
		K_{mPPi_Suc7} =0.11 mM	Nakano *et al.* (1989)
		K_{mUDPG_Suc7} =0.12mM	Nakano *et al.* (1989)
		K_{mUTP_Suc7} =0.1 mM	Nakano *et al.* (1989)
		K_{e_Suc7} =0.31 mM	Hansen *et al.* (1966).
2.4.1.14	Suc8	K_{iFBP_Suc8} =0.8 mM	Harbron *et al.* (1981)
		K_{iPi_Suc8} =11.0 mM	Harbron *et al.* (1981)
		K_{iSuc_Suc8} =50.0 mM	Salermo and Pontis (1978)
		K_{iSucP_Suc8} =0.4 mM	Harbron *et al.* (1981)
		K_{iUDP_Suc8} =0.7 mM	Harbron *et al.* (1981)
		K_{mF6P_Suc8} =0.8 mM	Lunn and Rees (1990)
		K_{mUDPG_Suc8} =2.4 mM	Lunn and Rees (1990)
		K_{e_Suc8} =10.0	Lunn and Rees (1990)
3.1.3.24	Suc9	K_{mSuc_Suc9} =80.0 mM	Cumino (2001)
		K_{mSucP_Suc9} =0.35 mM	Whitaker (1984)
		K_{e_Suc9} =780.0	Zhu *et al.* (2007)

2.7.1.105	Suc3	K_{iADP_Suc3} =0.16 mM	Kretschmer and Hofmann (1984)
		K_{iDHAP_Suc3} =0.7 mM	Markham and Kruger (2002)
		K_{mATP_Suc3} =0.5 mM	Walker and Huber (1987), Markham and Kruger (2002)
		K_{mF26BP_Suc3} =0.021 mM	Garcia de Frutos and Baanante (1995)
		K_{mF6P_Suc3} =0.5 mM	Walker and Huber (1987), Markham and Kruger (2002)
		K_{e_Suc3} =590.0	Cornish-Bowden (1997)
3.1.3.46	Suc4	K_{iF6P_Suc4} =0.1 mM	Villadsen and Nielsen (2001)
		K_{iPi_Suc}4 =0.5 mM	Villadsen and Nielsen (2001)
		K_{mF26BP_Suc4}= 0.032 mM	Macdonald *et al.* (1989)
5.3.1.9	Sta1	K_{e_Sta1}=2.3	Bassham and Krause (1969)
5.4.2.2	Sta2	K_{e_Sta2}=0.058	Colowick and Sutherland (1942)
2.7.7.27	Sta3	K_{aPGA_Sta1}=0.2252 mM	Assumed
		K_{mG1P_Sta3}=0.038 mM	Fuchs *et al.* (1979)
		K_{mATP_Sta3}=0.12 mM	Boehlein *et al.* (2005)
		$K_{iPi\_ATP\_Sta3}$=2.96 mM	Boehlein *et al.* (2005)
		K_{mPPi_Sta3}=0.033 mM	Amir *et al.* (1972)
		$K_{iCPP1\_ATP\_Sta3}$=13.8E-4 mM	Amir *et al.* (1972)
		K_{mADPG_Sta3}=0.24 mM	Sowokinos (1981)
		$K_{iADP\_ATP\_Sta3}$=2.0 mM	Ghosh *et al.* (1966)
		K_{e_Sta3}=1.1	Espada (1962)
3.6.1.1	Sta4	K_{mPPi_Sta2}=0.154 mM	Van *et al.* (2005)

		K_{e_Sta2}=1.57 E-4 mM	Flodgaard *et al.* (1974)
2.4.1.21	Sta5	K_{mADPG_Sta3}=0.077 mM	Hawker *et al.* (1974)
PGASink	PGAsink	$K_{mPGA\_PGASink}$=2.4 mM	Assumed, Zhu *et al.* (2007)
4.1.1.39PR	PR1	K_{mCO2_PR1}=0.0162 mM	Cousins *et al.* (2010)
		K_{mO2_PR1}=0.222 mM	Cousins *et al.*(2010)
		K_{mRuBP_PR1}=0.02 mM	Farquhar (1979)
		K_{iPGA_PR1}=2.52 mM	Assumed Badger and Lorimer (1981)
		K_{iFBP_PR1}=0.04 mM	Badger and Lorimer (1981)
		K_{iSBP_PR1}=0.75 mM	Badger and Lorimer (1981)
		K_{iPi_PR1}=3.6 mM	Assumed Badger and Lorimer (1981)
		K_{iNADPH_PR1}=0.21 mM	Assumed Badger and Lorimer (1981)
3.1.3.18	PR2	K_{mPGCA_PR2}=0.026 mM	Christeller and Tolbert (1978)
		K_{iPI_PR2}=2.55 mM	Christeller and Tolbert (1978)
		K_{iGCA_PR2}=94.0 mM	Christeller and Tolbert (1978)
1.1.3.15	PR3	K_{mGCA_PR3}= 0.1 mM	Tolbert (1981)
2.6.1.4	PR4	K_{e_PS4}= 607.0	Cooper and Meister (1972)
		K_{mGOA_PS4}=0.15 mM	Nakamura and Tolbert (1983)
		K_{mGLU_PS4}= 1.7 mM	Nakamura and Tolbert (1983)
		K_{iGLY_PS4}=2.0 mM	Zhu et al. (2007)
2.6.1.45	PR6	K_{e_PR6}= 0.24	Guynn (1982)
		K_{mGOA_PR6}=0.15 mM	Nakamura and Tolbert (1983)
		K_{mSER_PR6}=2.7 mM	Nakamura and Tolbert (1983)
		K_{iGLY_PR6}=33.0 mM	Nakamura and Tolbert (1983)

1.1.1.29	PR7	K_{e_PR7}= 2.5 E-5	Guynn (1982), Zhu et al (2007)
		K_{iHPR_PR7}= 12.0 mM	Kleczkowski and Edwards (1989)
		K_{mHPR_PR7}=0.09 mM	Kleczkowski and Edwards (1989)
2.7.1.31	PR8	K_{e_PR8}= 300.0	Kleczkowski *et al.* (1985)
		K_{mATP_PR8}= 0.21 mM	Kleczkowski *et al.* (1985)
		K_{mGCEA_PR8}=0.25 mM	Kleczkowski *et al.* (1985)
		K_{iPGA_PR8}=0.72 mM	Assumed, Zhu *et al.* (2007)
Gly_ser	PR5	K_{mGLY_PS5}= 6.0 mM	Douce *et al.* (2001)
		K_{iSER_PS5}=4.0 mM	Douce *et al.* (2001)
Tgca	PR9	K_{mGCA_PR9}= 0.2 mM	Howitz and McCarty (1985)
		K_{iGCEA_PR9}= 0.22 mM	Howitz and McCarty (1985)
Tgcea	PR10	K_{mGCEA_PR10}= 0.39mM	Howitz and McCarty (1986)
		K_{iGCA_PR10}= 0.28 mM	Howitz and McCarty (1986)
5.4.2.1&4.2.1.11	Ex	K_{mPGA_62} = 0.1 mM	Laisk and Edwards (2000)
		K_{mPEP_62} = 0.5 mM	Laisk and Edwards (2000)
		Ke_62=0.4302	Laisk and Edwards (2000)
3.6.3.14M	ATPM	K_{mADP_ATPM} =0.014 mM	Davenport and Mccarty (1986)
		K_{mATP_ATPM} =0.11 mM	Penefsky (1974)
		K_{mPi_ATPM} =0.3 mM	Aflalo and Shavit (1983)
		K_{e_ATPM} =5.734 mM-1	Bassham and Krause (1969), Laisk *et al.*(1989)
		X =0.667	Assumed light partition coefficient

		Y =0.6	Assumed Jmax partition coefficient, von Caemmerer (2000) with modification
		F =0.7225	von Caemmerer (2000) F=abs(1-f)
		θ=0.7	von Caemmerer (2000)
		D =1	von Caemmerer (2000) ATP/e- whole chain +Qcycle
3.6.3.14B	ATPB	K_{mADP_ATPB} =0.014 mM	Davenport and Mccarty (1986)
		KmPi_ATPB =0.11 mM	Penefsky (1974)
		KmATP_ATPB =0.3 mM	Aflalo and Shavit (1983)
		K_{e_ATPB} =5.734 mM^{-1}	Bassham and Krause (1969), Laisk et al.(1989)
		G =0.667	von Caemmerer (2000) ATP/e-
1.18.1.2M	NADPHM	K_{mNADP_NADPHM}=0.0072 mM	Shin (1972)
		K_{mNADPH_NADPHM}=0.036 mM	Gozzer *et al.* (1977)
		K_{e_NADPHM} =502	Knaff (1996), Keirns (1972), Laisk and Edwards (2000)
		E =0.5	von Caemmerer (2000)
Metabolite transport through Plasmodesmata	Leak	D_{CO2_PD}=1.7×10-9	Evans *et al.* (2009)
		l_{PD}=0.4µm	von Caemmerer and Furbank (2003)
		S_W/S_l=0.83	Sowinski *et al.* (2008)
		ϕ=0.03	Hatch and Osmond (1976); Stitt M, Heldt HW (1985b)
	TMAL	D_{MAL_PD}=6.67×10^{-10}	Sowinski et al (2008)
	TPYR	D_{PYR_PD}=7.00×10^{-10}	Sowinski et al (2008)

	TPGA	$D_{PGA\_PD}=5.25\times10^{-10}$	Sowinski et al (2008)
	TGAP	$D_{GAP\_PD}=5.25\times10^{-10}$	Sowinski et al (2008)
	TDHAP	$D_{DHAP\_PD}=5.25\times10^{-10}$	Sowinski et al (2008)
Leak_Bchl	Leak_Bchl	$P_{CO2\_m}=0.002$ cm s^{-1}	Evans et al (2009)
			Uehlein et al. (2008)
		$S_{Chl}/S_l=10$	Assumed
DiT1	TOAAM	$K_{m\_OAA\_M}=0.053$	Hatch *et al.* (1984)
		$K_{imal\_OAA\_M}=7.5$	Hatch *et al.* (1984)
	TmalM	$K_{m\_MAL\_M}=0.5$	Day and Hatch (1981)
		$K_{iOAA\_MAL\_M}=0.3$	Day and Hatch (1981)
DiT2	TmalB	$K_{m\_MAL\_B}=1$	Assumed, refer to parameters of DiT1
PPT	TPEPM	$K_{m\_PEP\_M}=0.3$	Assumed
MEPM	TpyrM	$K_{m\_PYR\_M}=0.05$	Assumed
MEPB	TpyrB	$K_{m\_PYR\_B}=0.05$	Assumed
TPTM	TPGAM	$K_{mPGA} = 2$	Assumed, Zhu *et al.* (2007) with modification
	TGAPM	$K_{mGAP} = 2$	Assumed, Zhu *et al.* (2007) with modification
	TDHAPM	$K_{mDHAP} = 2$	Assumed, Zhu *et al.* (2007) with modification
TPTB	TPGAB	$K_{mPGA} = 2$	Assumed, Zhu *et al.* (2007) with modification
	TGAPB	$K_{mGAP} = 2$	Assumed, Zhu *et al.* (2007) with modification
	TDHAPB	$K_{mDHAP} = 2$	Assumed, Zhu *et al.* (2007) with modification
Carbon isotope (^{13}CO$_2$)	Inf$_{\_h}$	$\alpha_0=1.0044$	16O'Leary (1984)
		$\alpha_1=1.0029$	Farquhar (1983)
	v_1	$\alpha_2=0.991$	Emrich et al. (1970); Mook et al.

calculation			(1974)
		$\alpha_{3=}$1.0011	Mook et al. (1974); O'Leary (1984)
	v_{2_h}	α_4=1.002	O'Leary *et al.* (1981)
	v_{6_h}	α_5=1.029	Roeske & O'Leary (1984)
	v_{leak_h}	α_6=1.0007	O'Leary (1984)
	R_{d_h}, $v_{pr\_5\_h}$	Δ_l=4	Farquhar (1983) standard carbon isotope discrimination of C4 plant

5.3 The volume of different compartments

Compartments	Parameters	Reference
MC cytosol	Vol_{Mcyto} =0.01 L m^{-2}	Different cell type proportions were measured from Maize leaf cross section and subcellular volumes was determined by reference to the measurement result of Barley leaf (Winter *et al.*, 1993)
MC chloroplast	Vol_{Mchl} =0.02 L m^{-2}	
BSC cytosol	Vol_{Bcyto} =0.0045 L m^{-2}	
BSC chloroplast	Vol_{Bchl} =0.009 L m^{-2}	
BSC peroxysome	Vol_{Bper} =0.00045 L m^{-2}	

5.4 Initial value of metabolite concentrations

Metabolite name	Concentration	Compartment	Reference
CO2	0.004	MC	Jenkins *et al.* (1989)
HCO3	0.077	MC	Jenkins *et al.* (1989)
OAA	0.1	MC	Assumed
PEP	2	MC	Stitt *et al.* (1985)
Malate	35	MC	Stitt *et al.* (1985)
Pyruvate	6	MC	Stitt *et al.* (1985)
PGA	4	MC	Stitt *et al.* (1985)
FBP	1.2	MC	Leegood (1985)
UDPG	0.6	MC	Zhu *et al.* (2007)

SUCP	0.0	MC	Assumed
SUC	0.0	MC	Assumed
F26BP	7.8E-6	MC	Zhu *et al.* (2007)
ATP	0.35	MC	Zhu *et al.* (2007)
T3P	11	MC	Stitt *et al.* (1985)
HexP	5	MC	Leegood, (1985)
Sucrose	0.0	MC	Assumed
OAA	0.05	Mchl	Assumed
Malate	35	Mchl	Stitt *et al.* (1985)
PEP	2	Mchl	Stitt *et al.* (1985)
Pyruvate	6	Mchl	Stitt *et al.* (1985)
NADPH	0.21	Mchl	Zhu *et al.* (2007), Giersch *et al.* (1980), Woodrow and Mott (1993)
ATP	0.68	Mchl	Zhu *et al.* (2007)
PGA	4	Mchl	Stitt *et al.* (1985)
T3P	11	Mchl	Stitt *et al.* (1985)
T3P	1	BSC	Stitt *et al.* (1985)
PGA	13	BSC	Stitt *et al.* (1985)
Malate	17	BSC	Stitt *et al.* (1985)
Pyruvate	5	BSC	Stitt *et al.* (1985)
CO_2	0.07	BSC	Jenkins *et al.* (1989)
CO_2	0.1	Bchl	Assumed
RuBP	2.0	Bchl	Zhu *et al.* (2007), Bassham and Krause (1969), Dietz and Heber (1984), Schimkat *et al.* (1990), Woodrow and Mott (1993)
PGA	13	Bchl	Stitt *et al.* (1985)
ATP	0.68	Bchl	Zhu *et al.* (2007)
NADPH	0.21	Bchl	Zhu *et al.* (2007), Giersch *et al.*

			(1980), Woodrow and Mott (1993)
SBP	0.15	Bchl	Zhu *et al.* (2007), Bassham and Krause (1969), Schimkat *et al.* (1990), Woodrow and Mott (1993)
S7P	0.25	Bchl	Zhu *et al.* (2007), Bassham and Krause (1969), Woodrow and Mott (1993)
FBP	0.3	Bchl	Leegood, (1985)
E4P	0.05	Bchl	Bassham and Krause (1969), Woodrow and Mott (1993)
Starch	0	Bchl	Assumed
T3P	1	Bchl	Stitt *et al.* (1985)
HexP	4	Bchl	Leegood (1985)
Pent	0.05	Bchl	Bassham and Krause (1969), Schimkat *et al.* (1990), Woodrow and Mott (1993)
Malate	17	Bchl	Stitt *et al.* (1985)
Pyruvate	5	Bchl	Stitt *et al.* (1985)
PGCA	0.0029	Bchl	Zhu *et al.* (2007)
GCA	0.36	Bchl	Zhu *et al.* (2007)
GCEA	0.181	Bchl	Zhu *et al.* (2007)
PPi	0	Bchl	Assumed
ADPG	0	Bchl	Assumed
GCA	0.36	Bper	Zhu *et al.* (2007)
GOA	0.028	Bper	Zhu *et al.* (2007)
GLY	1.8	Bper	Zhu *et al.* (2007)
SER	7.5	Bper	Zhu *et al.* (2007)
HPR	0.0035	Bper	Zhu *et al.* (2007)
GCEA	0.1812	Bper	Zhu *et al.* (2007)

5.5 Molecular weight and catalytic number of the enzymes in photosynthetic carbon metabolism

Enzyme Name	EC	Molecular Weight (D)	Catalytic number1 (s^{-1})	Reference
CA	4.2.1.1	160000	110000	Lazova *et al.* (2008) Yu *et al.* (2007)
PEPC	4.1.1.31	110000	66	Xu *et al.* (2006)
NADP-MDH	1.1.1.82	143000	1520	Agostino *et al.* (1992) Lemaire *et al.* (1996)
NADP-ME	1.1.1.40	226000	805.2	Detarsio *et al.* (2003)
PPDK	2.7.9.1	370000	144	Sugiyama. 1973 McGuire *et al.*. (1996)
Rubisco	4.1.1.39	532000	37.6	Reger *et al.* (1983) Cousins *et al.* (2010)
PGA Kinase	2.7.2.3	45000	540	Fifis and Scopes (1978), Bentahir *et al.* (2000)
GAP Dehydrogenase	1.2.1.12	180000	50	Speranza and Ferri (1982)
Aldolase	4.1.2.13	143000	65	Krueger and Sschnarrenberger (1983), Moorhead and Pplaxton (1990)
FBPase	3.1.3.11	160000	22.9	Tang *et al.* (2000), Reichert et al.(2000)
Transketolase	2.2.1.1	160000	69	Nilsson *et al.* (1998) Teige *et al.* (1989)
SBPase	3.1.3.37	66000	81	Cadet *et al.* (1988), Cadet *et al.* (1987)
PRK	2.7.1.19	90000	615	Surek *et al.* (1985), Porter *et al.* (1986)
ADPG Pyrophospho-rylase	2.7.7.27	210000	546	Kleczkowski *et al.* (1991), Li and Preiss (1992)
Phosphoglycolate phosphatase	3.1.3.18	100000	292	Kim *et al.* (2004), Kerr and Gear (1974)
Glycerate Kinase	2.7.1.31	47000	200	Kleczkowski *et al.* (1985), Kleczkowski and Randall (1988)
Glycolalate oxidase	1.1.1.79	125000	437	Kleczkowski *et al.* (1986), Zelitch (1955)
Serine Glyoxylate aminotransferase	2.6.1.45	85000	97	Ireland and Joy (1983), Paszkowski and

				Niedzielsa (1990)
Glycerate dehydrogenase	1.1.1.29	90000	1629	Julliard and Breton-Gilet (1997), Izumi *et al.*(1990)
Glutamate Glyoxylate aminotransferase	2.6.1.44	70800	54	Paszkowski and Niedzielska (1989)
Glycine decarboxylase	1.4.4.2	270000	18	Hiraga and Kikuchi (1980), Kochi and Kikuchi (1974)
6-phosphofructo-2-kinase	2.7.1.105	390000	9300	Larondelle *et al.* 1986, Baez *et al.* (2003)
fructose-2,6-bisphosphate 2-phosphatase	3.1.3.46	390000	1550	Pilkis *et al.* (1987), Villadsen and Nielsen (2001),
UDP Glucose pyrophosphorylase	2.7.7.9	53000	400	Gustafson and Gander (1972), Sowokinos *et al.* (1993)
Sucrose phosphate synthase	2.4.1.14	480000	640	Sonnewald *et al.* (1993)
Sucrose phosphatase	3.1.3.24	120000	2500	Echeverria and Salerno (1994), Lunn *et al.* (2000)

6 Additional explanations

6.2 Rationale underlying the choice of the default CO_2 permeability coefficient

The value of CO_2 chloroplast membrane permeability (P_{CO2_Chl}), which we used in the model, was considered to be too low for C3 plant and would lead to a negative photosynthesis below 150 ubar (Tholen and Zhu, 2011). While in the C4 system, P_{CO2_Chl} exhibited the opposite effect on A (Fig. S9), because increased the CO_2 chloroplast membrane permeability increased leakiness and decreased the CO_2 concentration around rubisco in BSC chloroplast, thus photorespiration enhanced and photosynthesis reduced. The influence of P_{CO2_Chl} on A in our C4 model was less conspicuous than that performed in C3 photosynthesis model.

6.1 Rationale underlying the choice of the rate equation used to calculate CO_2 uptake rates

The CO_2 assimilation rate (A) was calculated as:

$$A = v_c - 0.5 v_o - R_d \tag{18}$$

where v_c and v_o are the rates of RuBP carboxylation and oxygenation respectively. R_d is the rate of mitochondrial respiration. The default value for R_d is 1 µmol m^{-2} s^{-1} with the rate of respiration in both BSC (R_b) and MC (R_m) being equal as 0.5 µmol m^{-2} s^{-1}. This equation predicts the same photosynthetic CO_2 uptake rate.

In von Caemmerer's C4 model (von Caemmerer, 2000), CO_2 assimilation was calculated by two equations, besides Eqn. 18, the following equation was also used:

$$A = v_p - v_{Leak} - R_m \tag{19}$$

The minimal of Eqn. 18 and 19 determines the actual A. While in our model, both calculation methods always reach the same result. Because when we calculated A using the ODE model, all metabolite levels were in steady state, i.e. there is no changes of metabolite levels with time Therefore,

$$\frac{d[CO_2]_{Bchl}}{dt} = (v_{ME} - v_c - v_{leak\_Bchl}).\frac{1}{Vol_{Bchl}} = 0 \tag{S1}$$

$$\frac{d[CO_2]_{BSC}}{dt} = (v_{leak\_Bchl} + v_{PR5} + R_b - v_{leak}).\frac{1}{Vol_{Bcyto}} = 0 \tag{S2}$$

Eqn. (18) and (19) can be written as:

$$v_{ME} = v_c + v_{leak\_Bchl} \tag{S3}$$

$$v_{leak\_Bchl} = v_{leak} - v_{PR5} - R_b \tag{S4}$$

Because at the steady state, one RuBP oxygenation lead to release of 0.5 CO_2 in the photorespiratory process, i.e.:

$$v_{PR5} = 0.5 \cdot v_o \tag{S5}$$

In C4 shuttle, since at steady state, no metabolite accumulates, CO_2 fixed by PEPC was equal to CO_2 released by NADP-ME:

$$v_p = v_{ME} \tag{S6}$$

Therefore, Eqn. (19) can be re-written as:

$$A = v_p - v_{Leak} - R_m = v_c + v_{leak} - 0.5 \cdot v_o - R_b - v_{Leak} - R_m = v_c - 0.5 \cdot v_o - R_d$$

7 Reference

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