Supplemental Table S1. Comparison of light used by the photosystems at different incident light intensities (PPFD µmol s-1 m2) for two modelling scenarios

scenario 1: objective function = minimisation of sum of fluxes, no lower bound on light used; scenario 2: objective function = minimisation of light use. In both scenarios the model output was export of sugars and amino acids to the phloem and this output value was constrained so that the CO2 uptake rate into the model matched experimental data for net CO2 assimilation rate for each incident light intensity.

PPFD	Light used (scenario 1)	Light used (scenario 2)	scenario 1 / scenario 2
100	47.13	47.13	1
200	83.87	83.86	1
300	119.94	118.34	1.01
400	153.02	149.98	1.02
500	184.12	179.37	1.03
600	211.78	205.93	1.03
700	237.29	230.23	1.03
800	259.85	251.7	1.03
900	280.03	270.92	1.03
1000	297.84	287.88	1.03
1100	312.68	302.01	1.04
1200	324.55	313.32	1.04
1300	334.64	322.93	1.04
1400	341.17	329.15	1.04
1500	345.92	333.67	1.04

Supplemental Table S2. Predicted relative use of linear- versus cyclic-electron transport in the chloroplast at different incident light intensities (PPFD).

The FBA model had an objective function of minimisation of sum of fluxes for a set out output rate of sugars and amino acids to the phloem (constrained so that the CO2 uptake rate into the model matched experimental data for net CO2 assimilation rate for each incident light intensity). Fluxes have units of µmol s-1 m2. Abbreviations: CET, cyclic electron transport; LET linear electron transport; PS, photosystem

Light PPFD	PSII e- flux	PSI e- flux	LET (fraction)	CET (fraction)
100	23.57	23.57	1	0
200	41.93	41.93	1	0
300	58.64	61.3	0.96	0.04
400	73.98	79.04	0.94	0.06
500	88.1	96.02	0.92	0.08
600	101.02	110.76	0.91	0.09
700	112.76	124.53	0.91	0.09
800	123.14	136.71	0.9	0.1
900	132.43	147.6	0.9	0.1
1000	140.63	157.21	0.89	0.11
1100	147.46	165.22	0.89	0.11
1200	152.92	171.63	0.89	0.11
1300	157.56	177.08	0.89	0.11
1400	160.57	180.6	0.89	0.11
1500	162.75	183.17	0.89	0.11

Supplemental Information S1. List of constraints common to all simulations

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####ADD CONSTRAINTS TO MODEL####
#Leaves - light: prevent uptake of organic substrates, force NO3 use rather than NH4
cobra_model.reactions.get_by_id("Sucrose_tx1").lower_bound=0
cobra_model.reactions.get_by_id("Sucrose_tx1").upper_bound=0
cobra_model.reactions.get_by_id("GLC_tx1").lower_bound=0
cobra_model.reactions.get_by_id("GLC_tx1").upper_bound=0
cobra_model.reactions.get_by_id("CO2_tx1").lower_bound=0
cobra_model.reactions.get_by_id("NH4_tx1").lower_bound=0
cobra_model.reactions.get_by_id("NH4_tx1").upper_bound=0
#Leaves - dark: prevent uptake of organic substrates and light
cobra_model.reactions.get_by_id("Sucrose_tx2").lower_bound=0
cobra_model.reactions.get_by_id("Sucrose_tx2").upper_bound=0
cobra_model.reactions.get_by_id("GLC_tx2").lower_bound=0
cobra_model.reactions.get_by_id("GLC_tx2").upper_bound=0
cobra_model.reactions.get_by_id("Photon_tx2").lower_bound=0
cobra_model.reactions.get_by_id("Photon_tx2").upper_bound=0
cobra_model.reactions.get_by_id("NH4_tx2").lower_bound=0
cobra_model.reactions.get_by_id("NH4_tx2").upper_bound=0
cobra_model.reactions.get_by_id("CO2_tx2").upper_bound=0

#Set chloroplast G6P transporter and Starch Phosphorylase to 0
cobra_model.reactions.get_by_id("G6P_Pi_pc1").lower_bound=0
cobra_model.reactions.get_by_id("G6P_Pi_pc1").upper_bound=0
cobra_model.reactions.get_by_id("G6P_Pi_pc2").lower_bound=0
cobra_model.reactions.get_by_id("G6P_Pi_pc2").upper_bound=0
cobra_model2.reactions.get_by_id("RXN0_5184_p1").lower_bound=0
cobra_model2.reactions.get_by_id("RXN0_5184_p1").upper_bound=0
cobra_model2.reactions.get_by_id("RXN0_5184_p2").lower_bound=0
cobra_model2.reactions.get_by_id("RXN0_5184_p2").upper_bound=0

#Turn off plastid terminal oxidase
cobra_model.reactions.get_by_id("Plastoquinol_Oxidase_p1").lower_bound=0
cobra_model.reactions.get_by_id("Plastoquinol_Oxidase_p1").upper_bound=0

#nitrate uptake constrained to 3:2 day:night
Nitrate_balance = Metabolite("Nitrate_bal_c", name = "Weights to balance nitrate uptake", compartment =
"c1")
cobra_model.reactions.get_by_id("Nitrate_ec1").add_metabolites({Nitrate_balance:-2})
cobra_model.reactions.get_by_id("Nitrate_ec2").add_metabolites({Nitrate_balance:3})

#Rubisco carboxylase : oxygenase constrained to 3:1
Rubisco_balance = Metabolite("rubisco_bal_p1", name = "Weights to balance RuBP carboxygenase oxygenase
balance", compartment = "p1")
cobra_model.reactions.get_by_id("RXN_961_p1").add_metabolites({Rubisco_balance:3})
cobra_model.reactions.get_by_id("RIBULOSE_BISPHOSPHATE_CARBOXYLASE_RXN_p1").add_metabolites({Ru
bisco_balance:-1})

#generic ATPase and NADPH oxidase constraints for maintenance costs
Maintenance_constraint = Metabolite("ATPase_NADPHoxidase_constraint_c1",name =
"ATPase_NADPHoxidase_constraint_c1", compartment = "c1")
Maintenance_constraint2 = Metabolite("ATPase_NADPHoxidase_constraint_c2",name =
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"ATPase_NADPHoxidase_constraint_c2", compartment = "c2")
Maintenance_constraint3 = Metabolite("Light_dark_maintainence_constraint",name =
"Light_dark_maintainence_constraint", compartment = "c1")
cobra_model.reactions.get_by_id("ATPase_tx1").add_metabolites({Maintenance_constraint:1,Maintenance_c
onstraint3:1})
cobra_model.reactions.get_by_id("ATPase_tx2").add_metabolites({Maintenance_constraint2:1,Maintenance_
constraint3:-1})
cobra_model.reactions.get_by_id("NADPHoxc_tx1").add_metabolites({Maintenance_constraint:-3})
cobra_model.reactions.get_by_id("NADPHoxc_tx2").add_metabolites({Maintenance_constraint2:-3})
cobra_model.reactions.get_by_id("NADPHoxm_tx1").add_metabolites({Maintenance_constraint:-3})
cobra_model.reactions.get_by_id("NADPHoxm_tx2").add_metabolites({Maintenance_constraint2:-3})
cobra_model.reactions.get_by_id("NADPHoxp_tx1").add_metabolites({Maintenance_constraint:-3})
cobra_model.reactions.get_by_id("NADPHoxp_tx2").add_metabolites({Maintenance_constraint2:-3})

#constrain sucrose and starch storage
Sucorse_starch_balance = Metabolite("sucrose_starch_bal_c", name = "Weights to balance sucrose-starch
uptake", compartment = "c1")
cobra_model.reactions.get_by_id("SUCROSE_v_dielTransfer").add_metabolites({Sucorse_starch_balance:-90})
cobra_model.reactions.get_by_id("STARCH_p_dielTransfer").add_metabolites({Sucorse_starch_balance:10})

#Chloroplast enolase was not detected in Arabidopsis mesophyll tissue
cobra_model.reactions.get_by_id("2PGADEHYDRAT_RXN_p1").lower_bound=0
cobra_model.reactions.get_by_id("2PGADEHYDRAT_RXN_p1").upper_bound=0
cobra_model.reactions.get_by_id("2PGADEHYDRAT_RXN_p2").lower_bound=0
cobra_model.reactions.get_by_id("2PGADEHYDRAT_RXN_p2").upper_bound=0

#Setting chloroplastic NADPH dehydrogenase to 0 ((Yamamoto et al., 2011)
cobra_model.reactions.get_by_id("NADPH_Dehydrogenase_p1").lower_bound=0
cobra_model.reactions.get_by_id("NADPH_Dehydrogenase_p1").upper_bound=0
cobra_model.reactions.get_by_id("NADPH_Dehydrogenase_p2").lower_bound=0
cobra_model.reactions.get_by_id("NADPH_Dehydrogenase_p2").upper_bound=0

#ATP_ADP_Pi constrained to 0 during the day because while there is evidence for its existance (NTT), it does
not carry high during the day
cobra_model.reactions.get_by_id("ATP_ADP_Pi_pc1").lower_bound = 0
cobra_model.reactions.get_by_id("ATP_ADP_Pi_pc1").upper_bound = 0

#turn off chlorophyll a/b cycling for energy dissipation
cobra_model.reactions.get_by_id("RXN_7674_p1").lower_bound = 0
cobra_model.reactions.get_by_id("RXN_7674_p1").upper_bound = 0

#turn off cytosolic ethanol-ethanal cycle for NADH dissipation
cobra_model.reactions.get_by_id("RXN_10745_NAD_c1").lower_bound = 0
cobra_model.reactions.get_by_id("RXN_10745_NAD_c1").upper_bound = 0

#turn off cytosolic ferric chelate reductase cycle for NADH dissipation
cobra_model.reactions.get_by_id("FERRIC_CHELATE_REDUCTASE_RXN_c1").lower_bound = 0
cobra_model.reactions.get_by_id("FERRIC_CHELATE_REDUCTASE_RXN_c1").upper_bound = 0

#Adding a H_mc reaction to allow protons into mitochondria
for i in range(1,3):
        rxn = Reaction("H_mc"+str(i))
        rxn.add_metabolites({cobra_model.metabolites.get_by_id("PROTON_c"+str(i)):-
1,cobra_model.metabolites.get_by_id("PROTON_m"+str(i)):1})
        rxn.lower_bound=0
        rxn.upper_bound=1000
cobra_model.add_reactions({rxn})
```