Supplemental information

Figure S1: Fit of phenological stages for APSIM and SIMPLACE against experimental data.

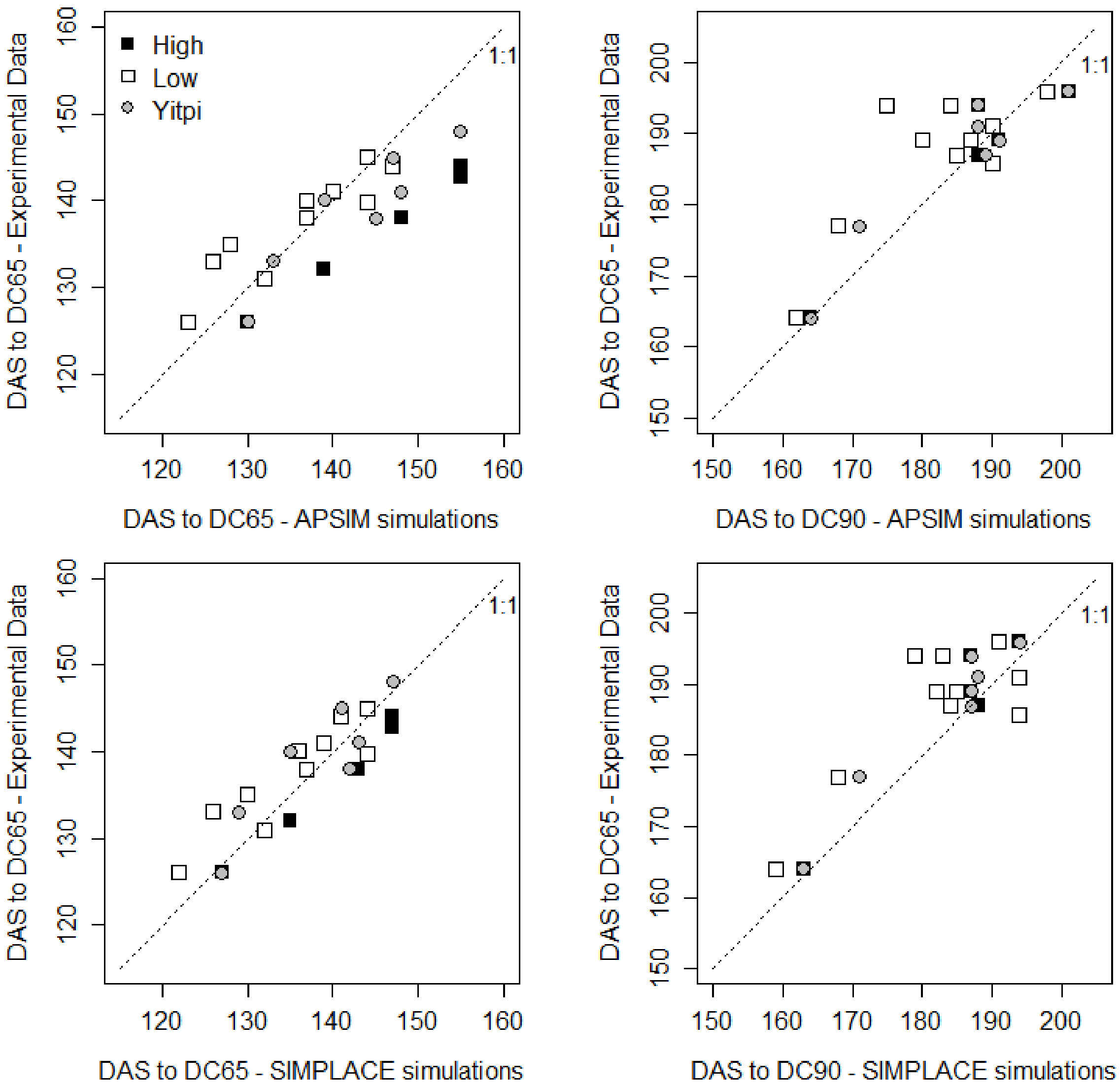

Figure S2: Range of specific leaf area (SLA) values of experimental data (AGFACE) and simulated data for both models with modifications for early vigour in the high and low vigour lines as described in Table 3.

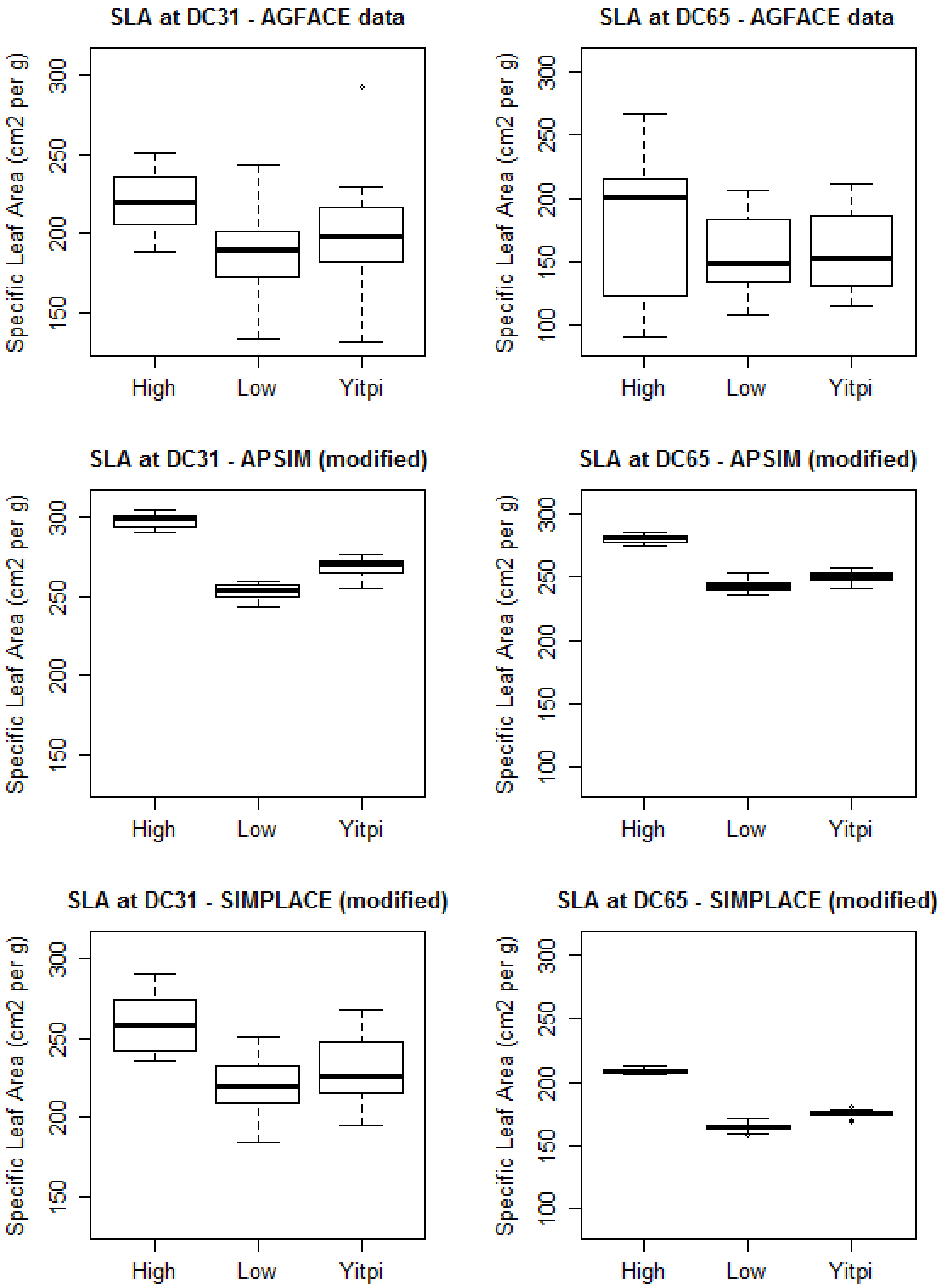

Figure S3: Range of leaf area index values (LAI) values of experimental data (AGFACE) and simulated data for both models with modifications for early vigour in the high and low vigour lines as described in Table 3.

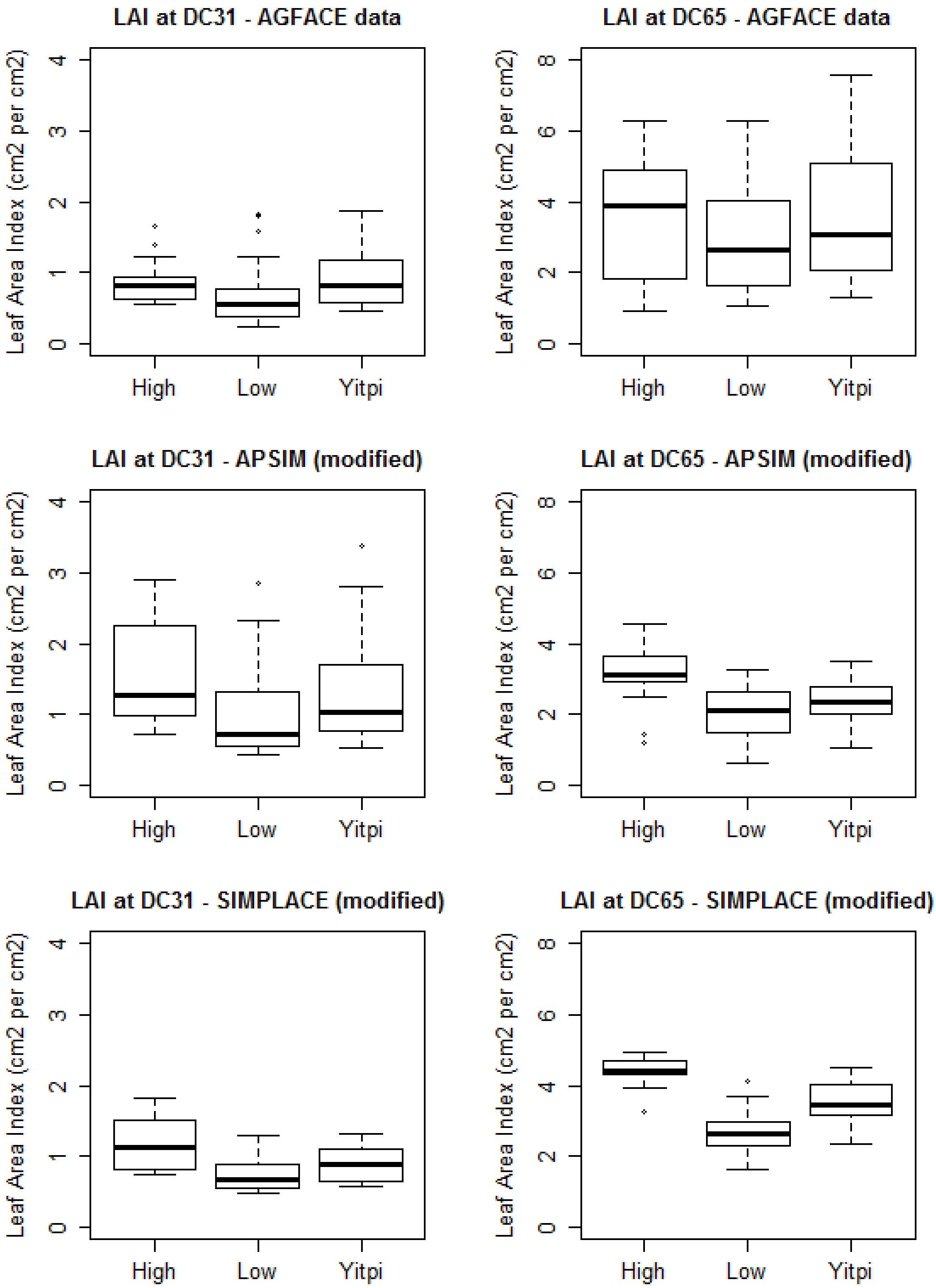

Figure S4: Fit of experimental AGFACE data to simulated results for leaf area index and above-ground biomass at stem elongation (DC31) for APSIM and SIMPLACE based on date of sampling. The group on the left higher than the 1:1 line is data from 2008, while the diffuse group underneath the 1:1 line with APSIM simulations is 2007 and 2009 (both planted late).

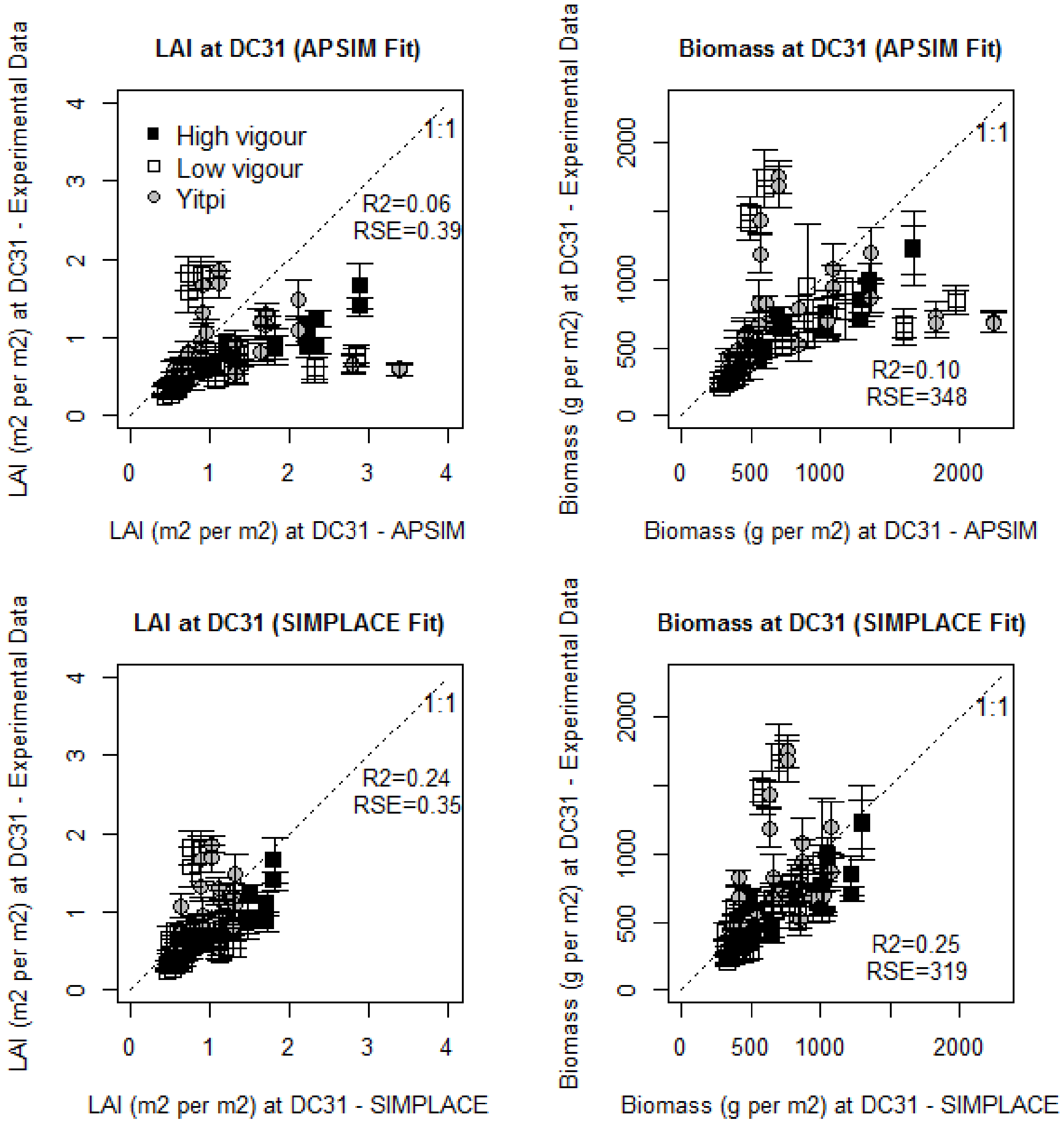

Figure S5: Simulated grain yield response to elevated [CO_2] according to vigour groups in different environment types (with characterization done with respective model) for the Australian Grains Free Air CO2 Enrichment (AGFACE) facility in 2007 to 2013. Simulated data includes all 7 cultivars in all 7 years, plus/minus irrigation (therefore including combinations that did not occur experimentally).

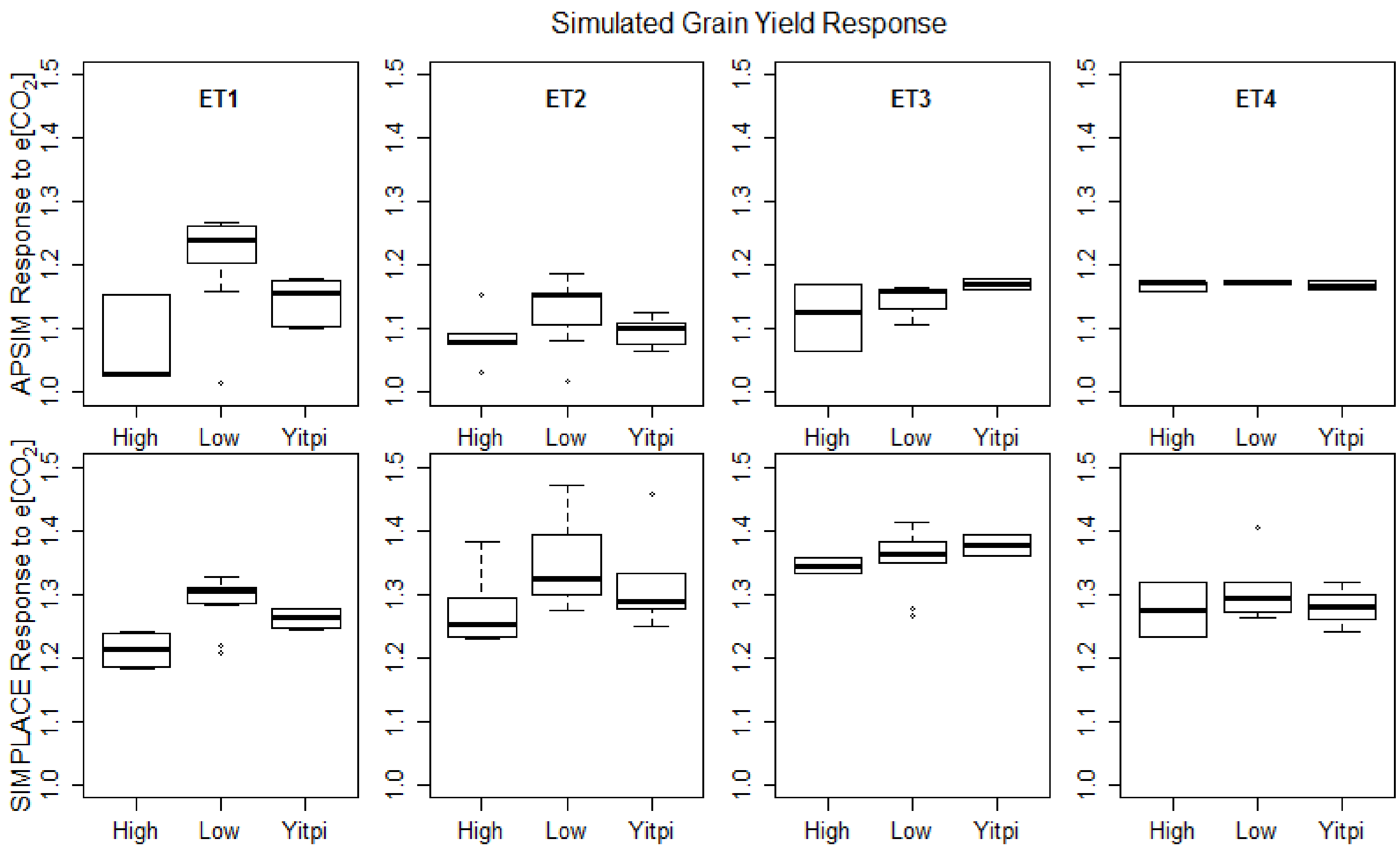

Figure S6: Simulated biomass response to elevated [CO_2] according to vigour groups in different environment types (with characterization done with respective model) for the Australian Grains Free Air CO2 Enrichment (AGFACE) facility in 2007 to 2013. Simulated data includes all 7 cultivars in all 7 years, plus/minus irrigation (therefore including combinations that did not occur experimentally).

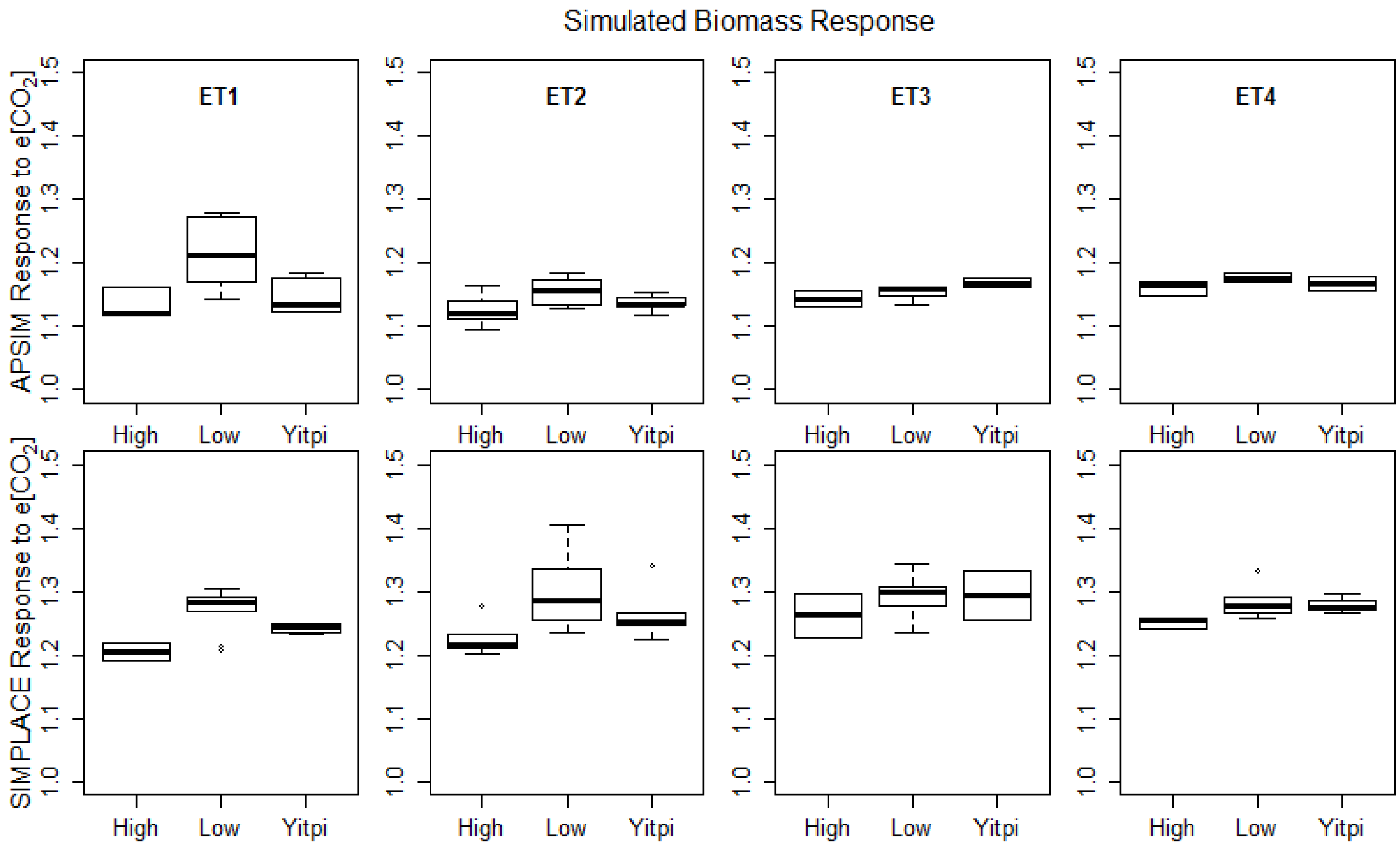

Figure S7: Correlations between relative simulated responses to e[CO_2] for pre-anthesis leaf area index and cumulative pre-anthesis water use, and between cumulative pre-anthesis water use and average post-anthesis water stress index. Relative responses are calculated as the simulated e[CO_2] values divided by ambient [CO_2] values. Water use is calculated as the sum of evaporation and transpiration, and cumulative pre-anthesis water use is the sum of daily values up to and including simulated anthesis (DC65). Leaf area index values used in the response are the daily values the day of simulated anthesis. The water stress index is calculated differently for each model: in APSIM (top row), this is calculated from the ratio of the soil water supply to crop water demand (with an upper bound of 1), while in SIMPLACE (bottom row) this is the ratio of actual transpiration to potential transpiration (TRANRF parameter). Values were averaged over the pre-anthesis period to account for different development times and higher values in the relative response refer to situations when the stress was lower with e[CO_2] compared to a[CO_2]. All high vigour lines are represented by the cultivar 'Hartog' as they did not differ in phenology or any other model parameters.

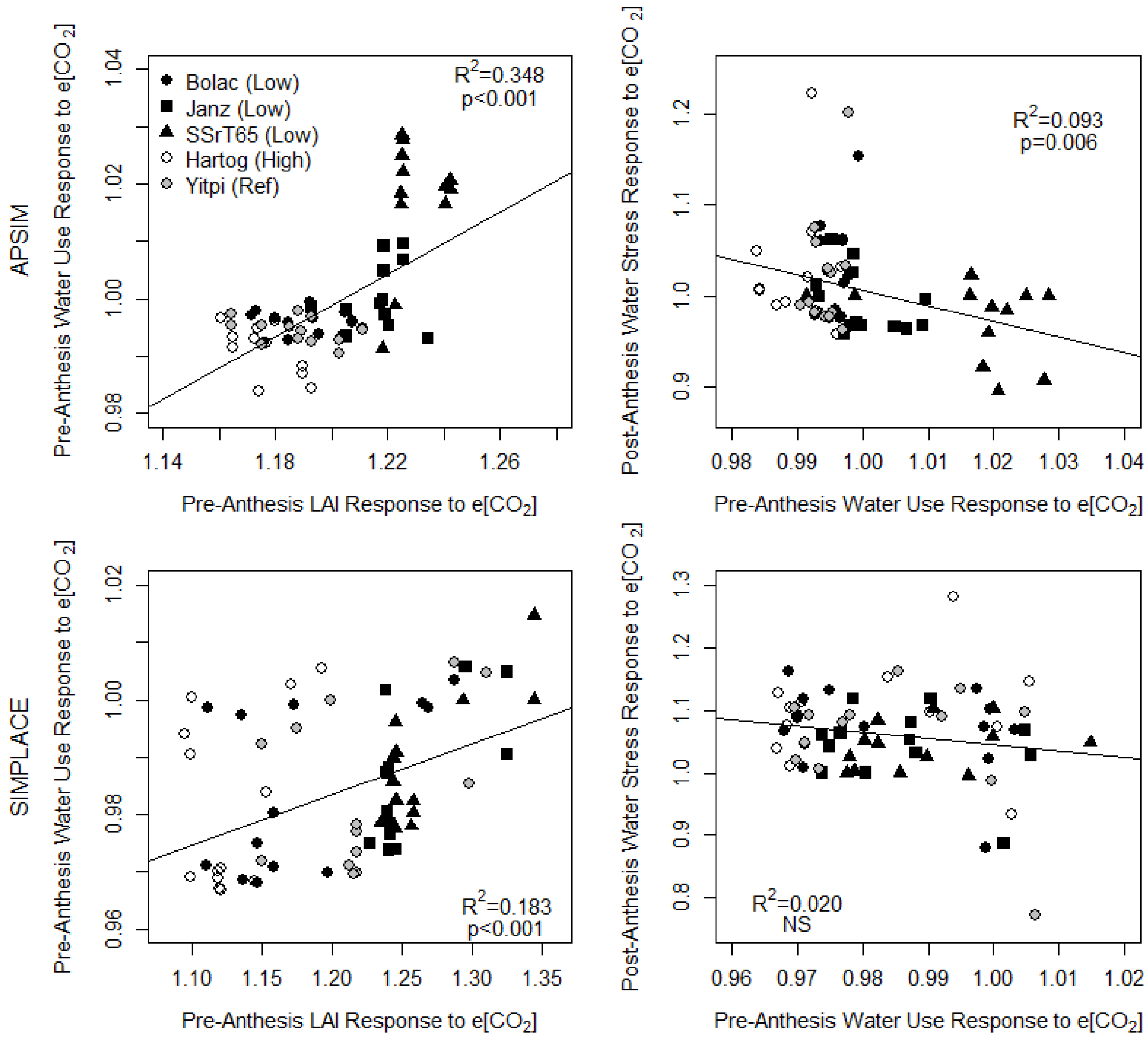
APSIM
SIMPLACE
Bolac (Low)
Janz (Low)
SSrT65 (Low)
Hartog (High)
Yitpi (Ref)
R^2=0.348
p<0.001
R^2=0.093
p=0.006
R^2=0.183
p<0.001
R^2=0.020
NS
Pre-Anthesis Water Use Response to e[CO_2]
Post-Anthesis Water Stress Response to e[CO_2]
Pre-Anthesis LAI Response to e[CO_2]
Pre-Anthesis Water Use Response to e[CO_2]

Figure S8: Correlations between relative simulated responses to e[CO_2] for average post-anthesis water stress index and cumulative pre-anthesis radiation intercepted with the simulated relative response in grain yield. Relative responses are calculated as the simulated e[CO_2] values divided by ambient [CO_2] values. Pre-anthesis values refer to values from planting to anthesis inclusively, while post-anthesis refers to the day after anthesis until maturity. The water stress index is calculated differently for each model: in APSIM (top row), this is calculated from the ratio of the soil water supply to crop water demand (with an upper bound of 1), while in SIMPLACE (bottom row) this is the ratio of actual transpiration to potential transpiration (TRANRF parameter). Daily values were averaged over the post-anthesis period (i.e the day after anthesis to maturity) to account for different development times. Higher values in the relative response refer to situations when the stress was lower with e[CO_2] compared to a[CO_2]. All high vigour lines are represented by the cultivar ‘Hartog’ as they did not differ in phenology or any other model parameters.

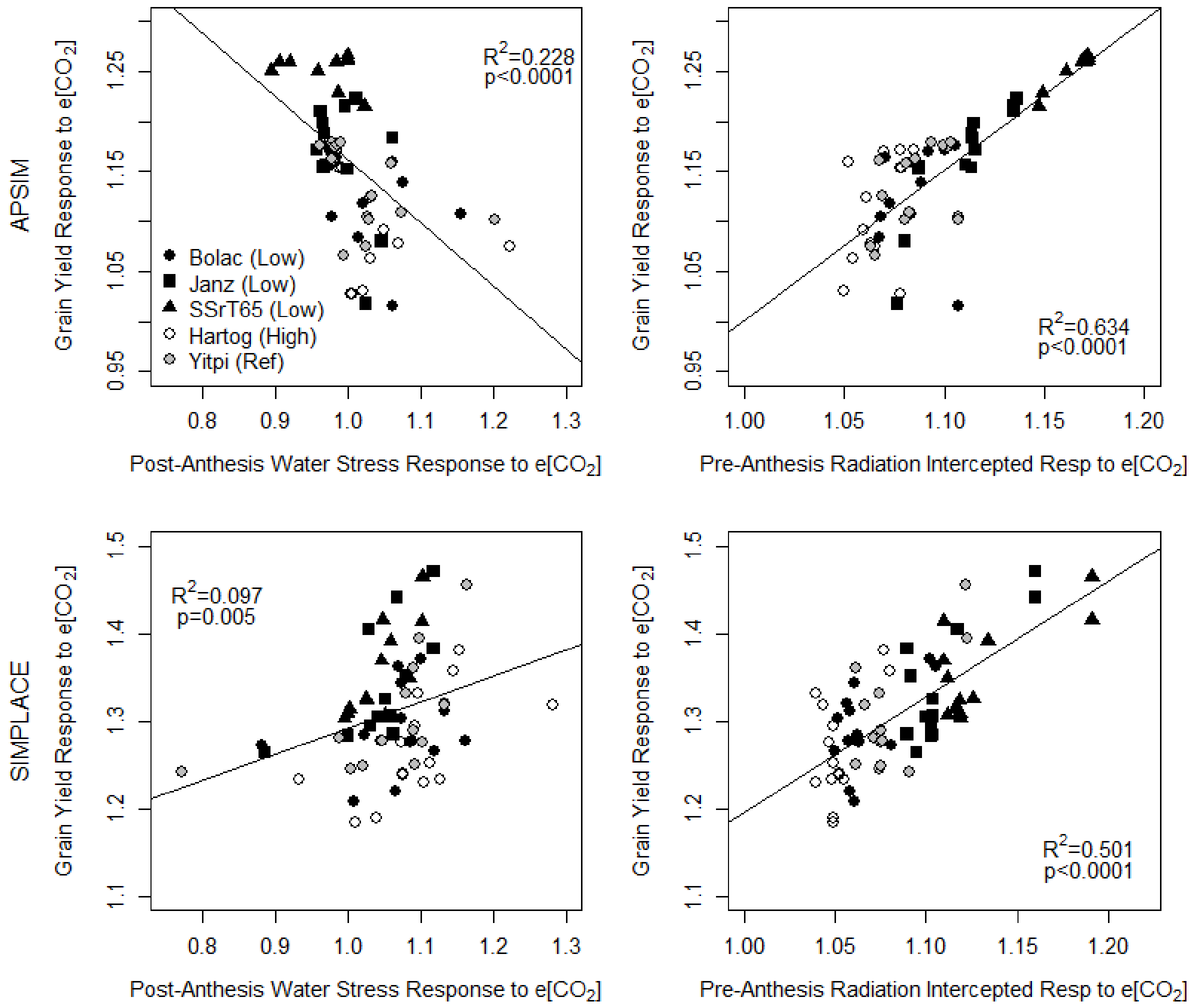
APSIM
SIMPLACE
Grain Yield Response to e[CO2]
Post-Anthesis Water Stress Response to e[CO2]
Pre-Anthesis Radiation Intercepted Resp to e[CO2]
R2=0.228
p<0.0001
R2=0.634
p<0.0001
R2=0.097
p=0.005
R2=0.501
p<0.0001
Bolac (Low)
Janz (Low)
SSrT65 (Low)
Hartog (High)
Yitpi (Ref)
0.95
1.05
1.15
1.25
1.1
1.2
1.3
1.4
1.5
0.8
0.9
1.0
1.1
1.2
1.3
1.00
1.05
1.10
1.15
1.20

Table S1: Soil profile parameters describing air dry, crop lower limit (LL), drained upper limit (DUL), saturation (SAT), bulk density (BD), pH, and organic carbon concentration (OC) of the experimental site used by both models. The wheat module in APSIM also uses additional water extraction coefficients (KL and XF), and SIMPLACE uses van Genuchten parameters related to water retention in unsaturated soils (alfa and n).

Depth (cm)	Air dry (g/cm^3)	LL (g/cm^3)	DUL (g/cm^3)	SAT (g/cm^3)	BD (g/cm^3)	pH	OC (%)	APSIM KL	APSIM XF	SIMPLACE ALFA	SIMPLACE N
0-10	0.15	0.20	0.39	0.46	1.14	8.4	1.248	0.06	1.00	1	1.23
10-20	0.18	0.23	0.40	0.47	1.30	8.4	0.708	0.06	1.00	1	1.23
20-40	0.25	0.27	0.42	0.48	1.37	8.9	0.354	0.04	1.00	1	1.23
40-60	0.27	0.30	0.43	0.47	1.40	9.0	0.177	0.02	0.80	1	1.23
60-80	0.28	0.33	0.45	0.47	1.40	9.0	0.089	0.02	0.80	1	1.23
80-100	0.30	0.35	0.45	0.47	1.40	9.0	0.044	0.02	0.60	1	1.23
100-120	0.32	0.36	0.45	0.47	1.40	9.0	0.022	0.02	0.60	1	1.23
120-140	0.33	0.37	0.45	0.47	1.40	9.1	0.011	0.02	0.20	1	1.23
140-160	0.34	0.37	0.45	0.47	1.40	9.1	0.011	0.02	0.20	1	1.23
160-180	0.34	0.37	0.45	0.47	1.40	9.1	0.011	0.02	0.20	1	1.23

Table S2: Starting soil nitrate content used by both models for simulation of AGFACE experiments (2007-2013).

Depth (cm)	2007	2008	2009	2010	2011	2012	2013
0-10	42	34.8	13.3	38.4	47.2	25.7	19.3
10-20	25	26.6	26.1	23.8	23.3	14.6	8.4
20-40	15	21.4	27.5	24.3	12.7	11.2	11.4
40-60	13	21.4	27.5	22.8	12.7	11.2	11.4
60-80	6	11.8	10.5	22.8	20.4	20.1	15.2
80-100	2.5	11.8	10.5	11.7	20.4	20.1	15.2
100-120	2	2	2	11.7	2	2	2
120-140	1	1	1	1	1	1	1
140-160	1	1	1	1	1	1	1
160-180	0	0	0	0	0	0	0

Table S3: Starting soil water content used by both models for simulation of AGFACE experiments (2007-2013).

	2007	2008	2009	2010	2011		2012		2013	
Depth (cm)					Rain	Suppl	Rain	Suppl	Rain	Suppl
0-10	0.363	0.340	0.406	0.269	0.303	0.311	0.165	0.181	0.187	0.181
10-20	0.398	0.278	0.419	0.287	0.392	0.381	0.219	0.234	0.179	0.179
20-40	0.411	0.324	0.383	0.311	0.447	0.423	0.285	0.309	0.265	0.258
40-60	0.419	0.373	0.341	0.347	0.451	0.432	0.340	0.355	0.333	0.337
60-80	0.429	0.396	0.351	0.384	0.450	0.434	0.381	0.385	0.372	0.383
80-100	0.443	0.423	0.376	0.406	0.448	0.451	0.403	0.401	0.411	0.415
100-120	0.441	0.453	0.424	0.414	0.469	0.469	0.418	0.421	0.438	0.431
120-140	0.444	0.443	0.385	0.414	0.469	0.469	0.418	0.421	0.438	0.431
140-160	0.429	0.411	0.390	0.414	0.469	0.469	0.418	0.421	0.438	0.431
160-180	0.415	0.388	0.379	0.414	0.469	0.469	0.418	0.421	0.438	0.431

Table S4: Irrigation amounts and dates for the supplemental irrigation treatment used by both models for simulation of AGFACE experiments (2007-2013).

Year	Dates	Amount (mm)
2007	17 September	10
	24 September	10
	2 October	10
	8 October	10
	16 October	28
	14 November	28
2008	8 September	20
	25 September	20
2009	6 October	10
	22 October	30
	3 November	30
2010	6 October	30
	11 October	20
	22 October	30
2011	6 September	10
	12 September	20
	22 September	20
	10 October	20
	18 October	30
2012	11 September	30
	25 September	30
	10 October	30
	29 October	30
2013	No supplemental irrigation applied	

S5: Grain yield, above-ground biomass at maturity (DC90) and harvest index (HI) according to vigour group (high, low and the reference cultivar Yitpi) in the Australian Grains Free Air CO_2 Enrichment (AGFACE) facility in 2007-2013.

	High early vigour		Low early vigour		Yitpi	
	a[CO_2]	e[CO_2]	a[CO_2]	e[CO_2]	a[CO_2]	e[CO_2]
Grain yield (t ha-1)	4.30	5.25	4.12	5.23	4.66	5.72
Biomass (t ha-1)	11.7	14.6	11.1	14.0	12.5	15.9
HI (%)	36.2	35.0	37.0	36.9	36.8	35.8