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Modelling ozone-induced changes in wheat amino acids and protein quality using a process-based crop model

Jo Cook et al.

Correspondence to: Jo Cook (jo.cook@york.ac.uk)

Comparison of meteorological inputs for 2017 and 2018

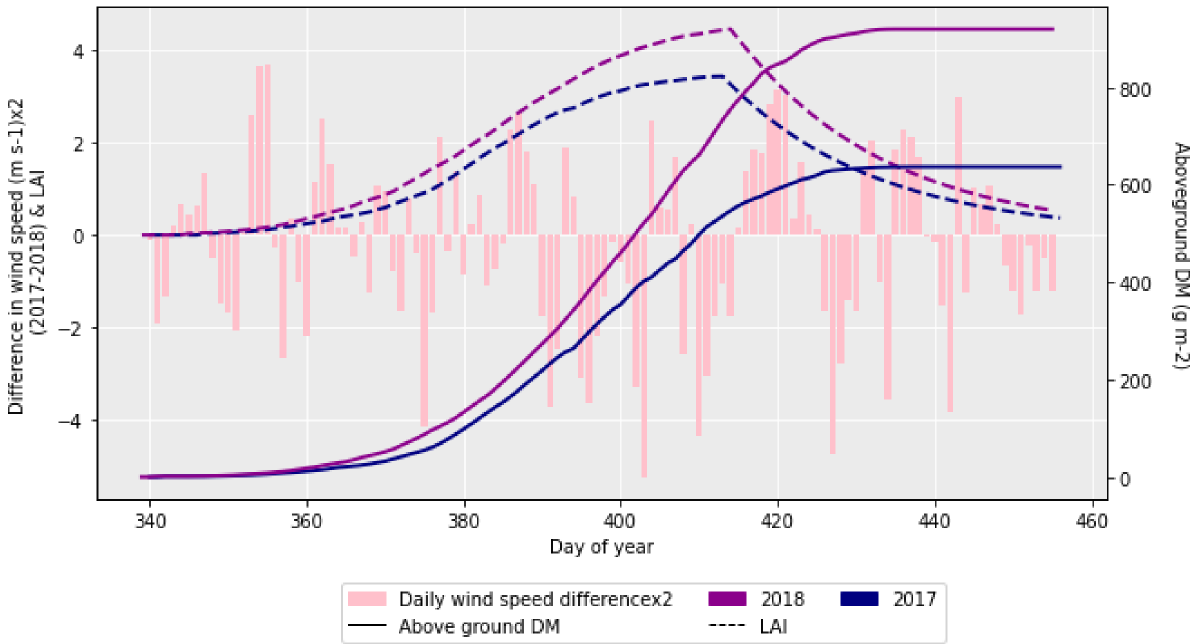

Fig S1: Daily mean difference in wind speed, where the wind speed for 2018 was subtracted from that for 2017, multiplied by 2, along with the difference in aboveground DM and LAI for the model run using the parameterisation noted "calibration method 2", which used all available data.

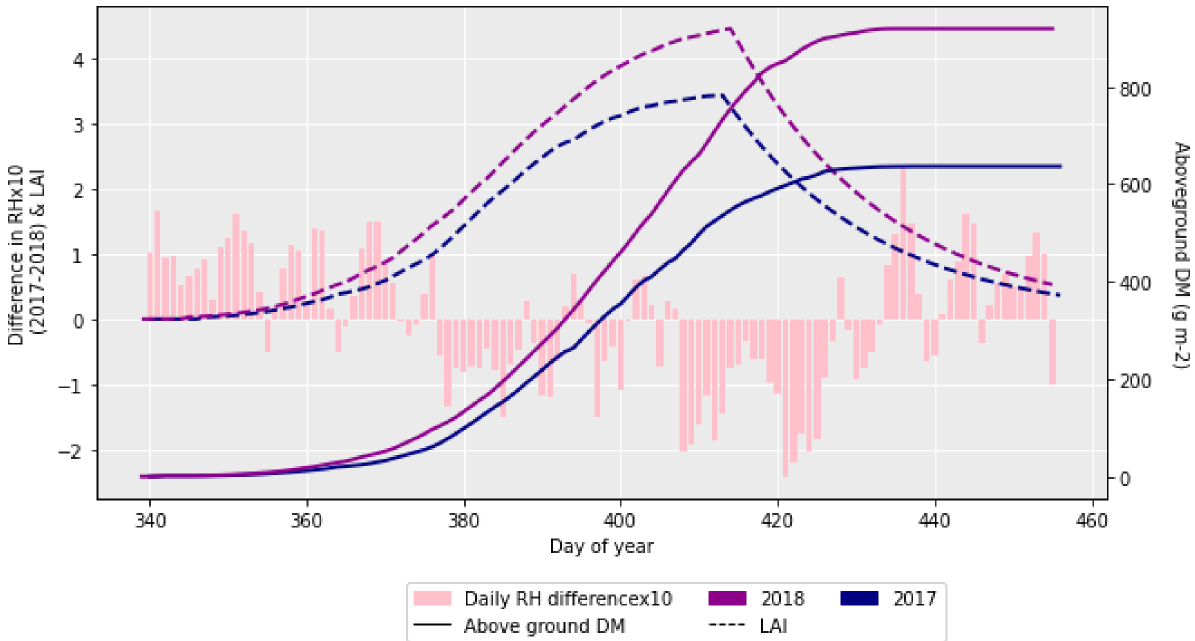

Fig. S2: Daily mean difference in RH, where the RH for 2018 was subtracted from that for 2017, multiplied by 10, along with the difference in aboveground DM and LAI for the model run using the parameterisation noted "calibration method 2", which used all available data.

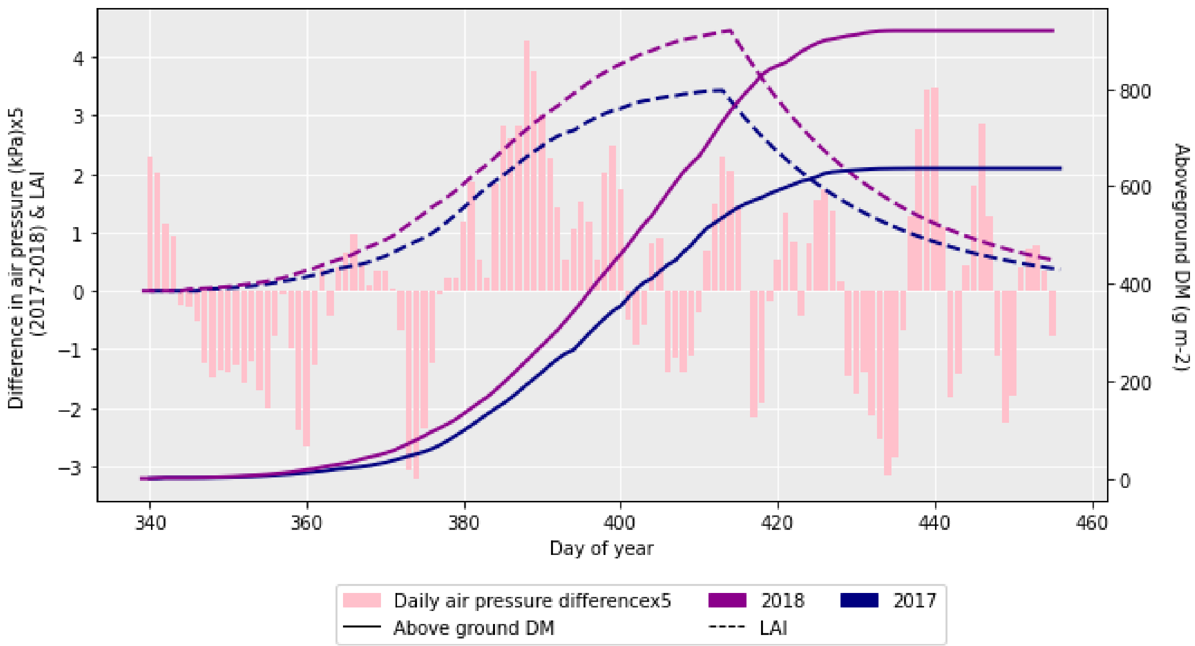

Fig. S3: Daily mean difference in air pressure, where the air pressure for 2018 was subtracted from that for 2017, multiplied by 5, along with the difference in aboveground DM and LAI for the model run using the parameterisation noted "calibration method 2", which used all available data.

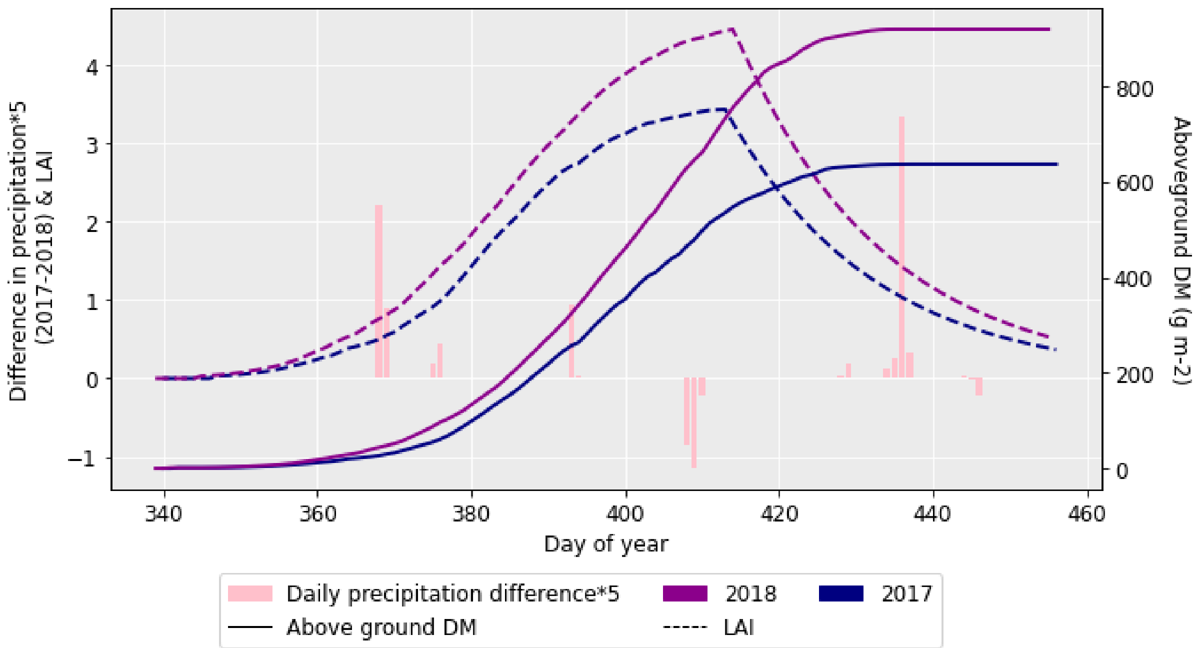

Fig. S4: Daily mean difference in precipitation, where the precipitation for 2018 was subtracted from that for 2017, multiplied by 5, along with the difference in aboveground DM and LAI for the model run using the parameterisation noted "calibration method 2", which used all available data. Wheat was assumed to be irrigated so lack of rain was not an issue in model runs

Comparison of photosynthetic processes

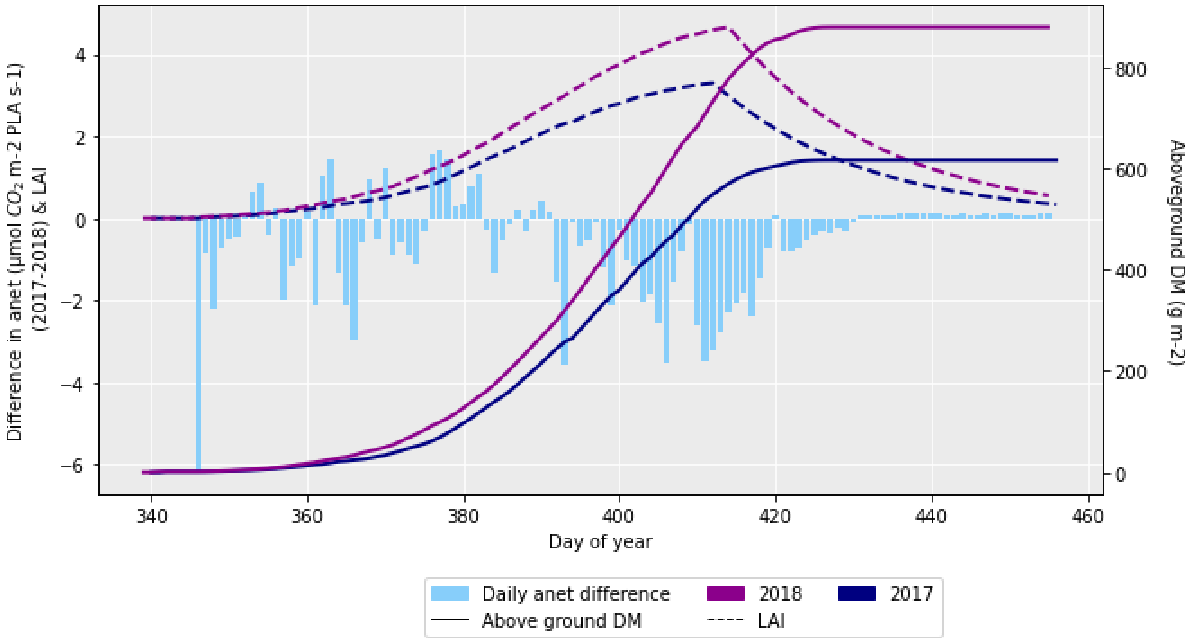

Fig. S5: The difference in net photosynthetic rate for 2017 and 2018, where the net photosynthetic rate for 2018 was subtracted from that for 2017, along with the difference in aboveground DM accumulation and LAI for the ambient treatment for the 2 years. The LAI and aboveground DM profiles are for the HD3118 cultivar.

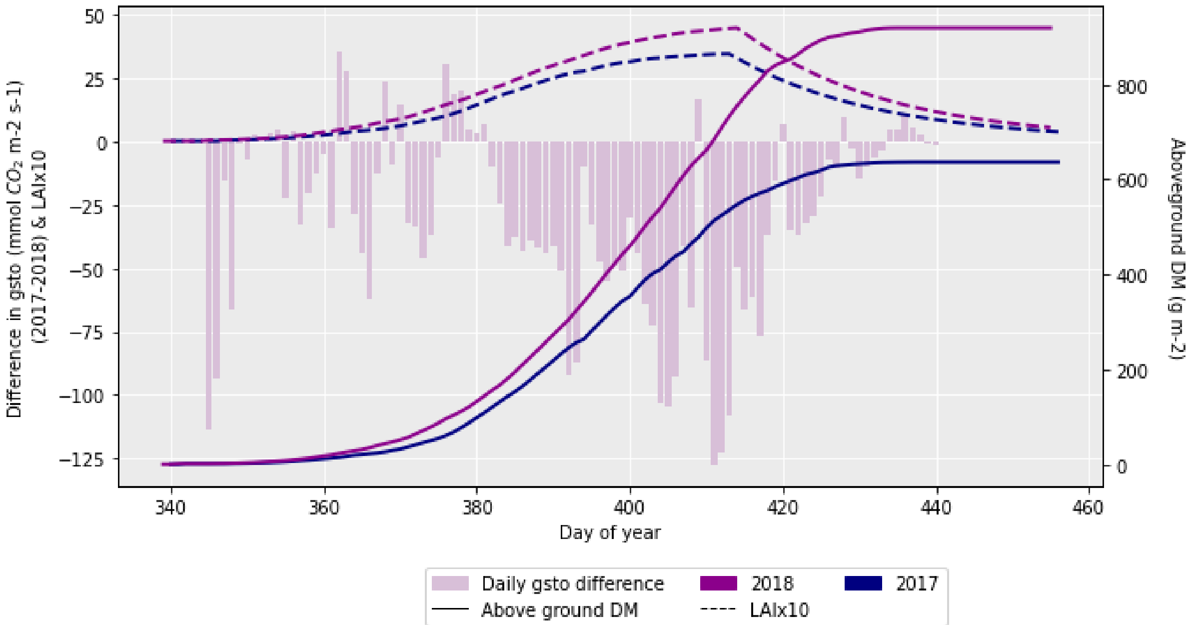

Fig. S6: The difference in sunlit stomatal conductance for 2017 and 2018, where the stomatal conductance for 2018 was subtracted from that for 2017, for the HUW234 cultivar along with the aboveground DM accumulation and LAI for both years. This run used the parameterisation of "calibration method 2" where all available data was used for calibration

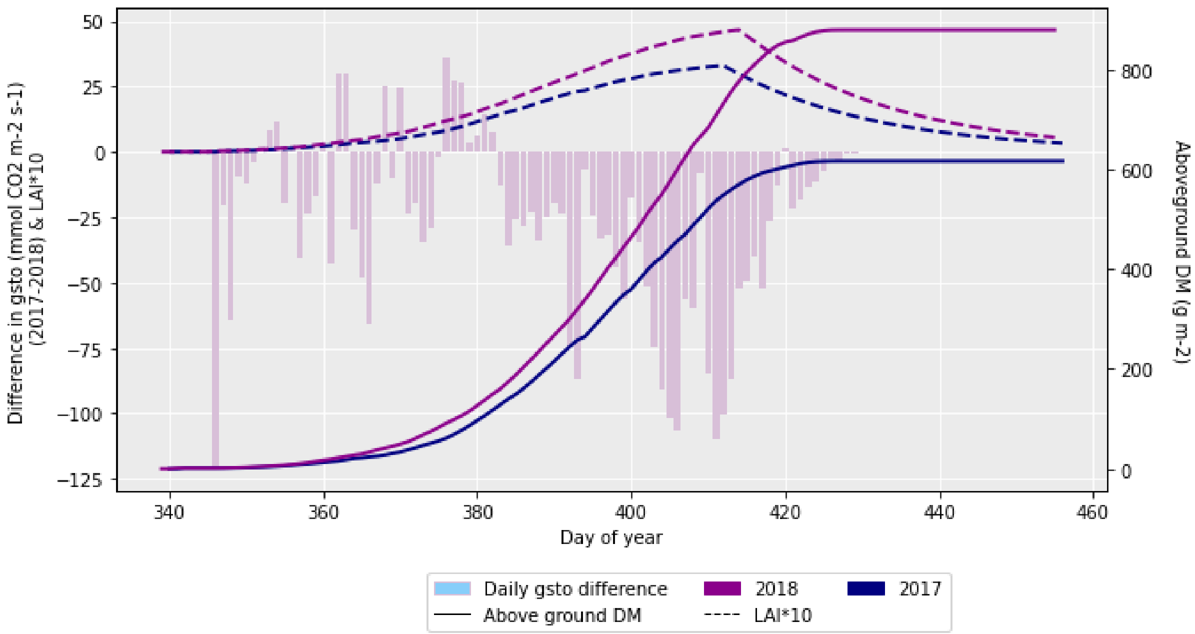

Fig. S7: The difference in sunlit stomatal conductance for 2017 and 2018, where the stomatal conductance for 2018 was subtracted from that for 2017, for the HD3118 cultivar along with the aboveground DM accumulation and LAI for both years. This run used the parameterisation of "calibration method 2" where all available data was used for calibration

Model calibration

Initially, the input data was split into 2 groups. The 2017 data was used to calibrate the model and the 2018 data was used to evaluate the model. However, with such limited data the 2017 calibration dataset was subject to overfitting and the parameterisation obtained in the calibration did not give good results for the 2018 evaluation dataset. The parameterisation using the 2017 data for calibration and 2018 for evaluation is referred to as calibration method 1, and the parameterisation used in the main body of the paper, which used all available data to develop a parameterisation, is referred to as calibration method 2.

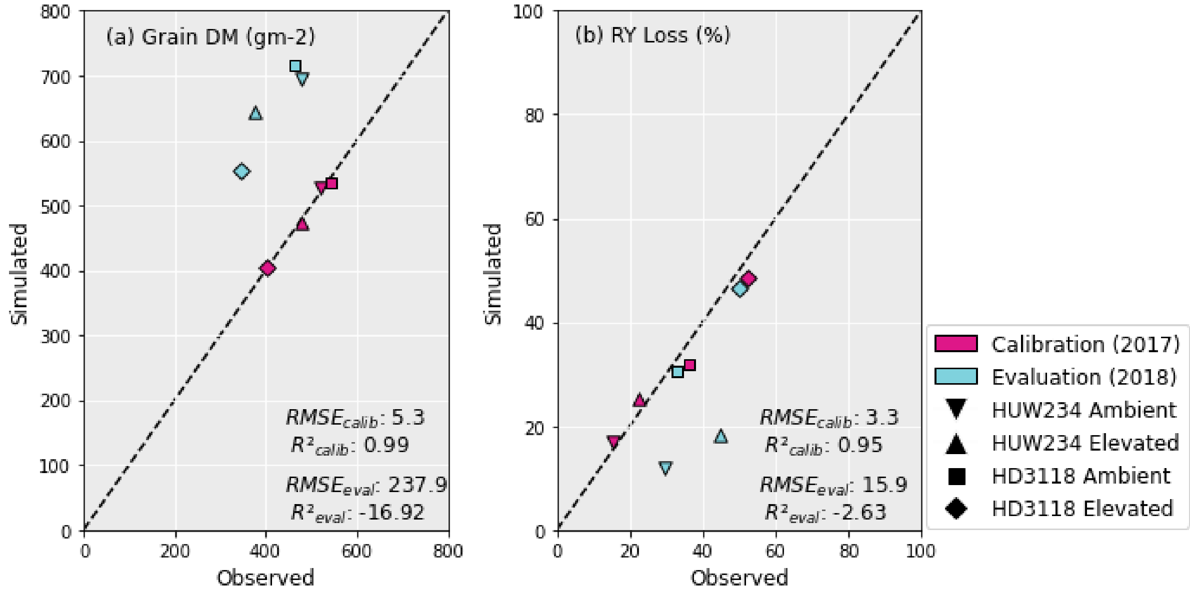

Figure S8: Calibration and evaluation of grain DM and RY loss using the DO$_3$SE-Crop model for the Varanasi dataset when using calibration method 1. RY loss was calculated comparative to preindustrial O_3 concentrations of 10 ppb (see main text – section 2.5).

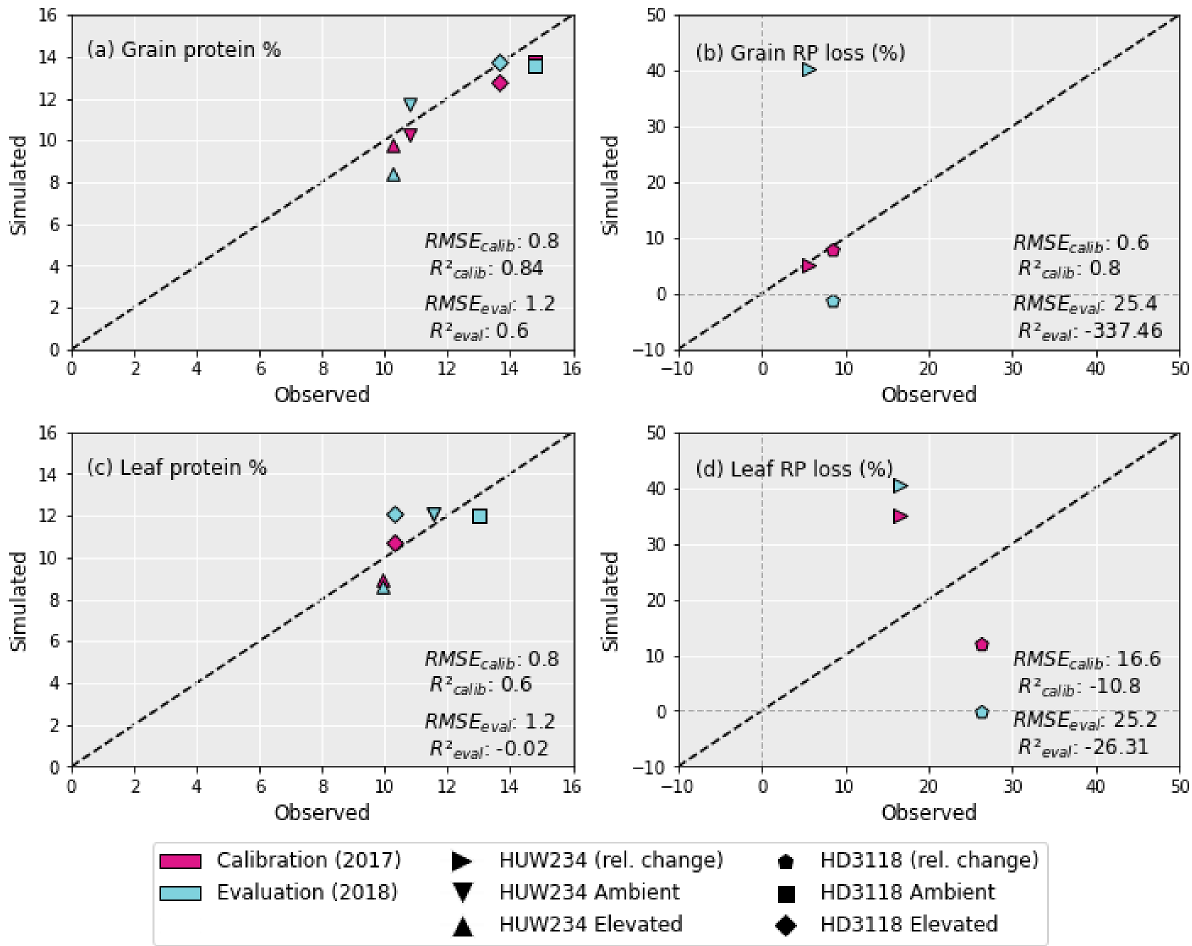

Fig. S9: Calibration and evaluation of the concentration of grain (a) and leaf (c) protein of HUW234 and HD3118 cultivars under ambient and elevated O_3. Calibration and evaluation of the relative change in grain (b) and leaf (d) protein percentage. In figure (c) the ambient leaf protein % for the HUW234 and HD3118 cultivars in the calibration and evaluation were almost identical, hence the overlaid points. RMSE and R^2 of both the calibration and evaluation are indicated on the plot. These results use calibration method 1.

Correcting for the heating effect of the open top chamber

Data on the internal chamber and ambient air temperatures in Delhi, over the course of the wheat growing season in December 2018 to March 2019 were regressed against each other to obtain a regression with which to correct the input temperature data in the present study, as the air temperature sensor was external to the chambers.

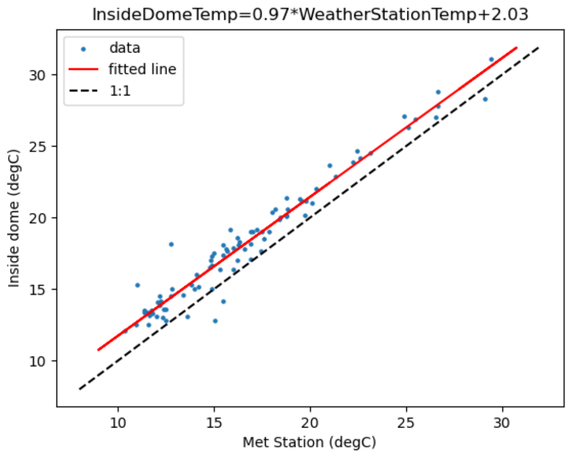

Figure S10: Regression between the air temperature as measured at the meteorological weather monitoring station and internal to the open top chambers in Delhi, during the wheat growth period 2018 to 2019. On average the open top chambers were approximately 2 degrees warmer than the ambient air.

O_3 profiles for 2017 and 2018

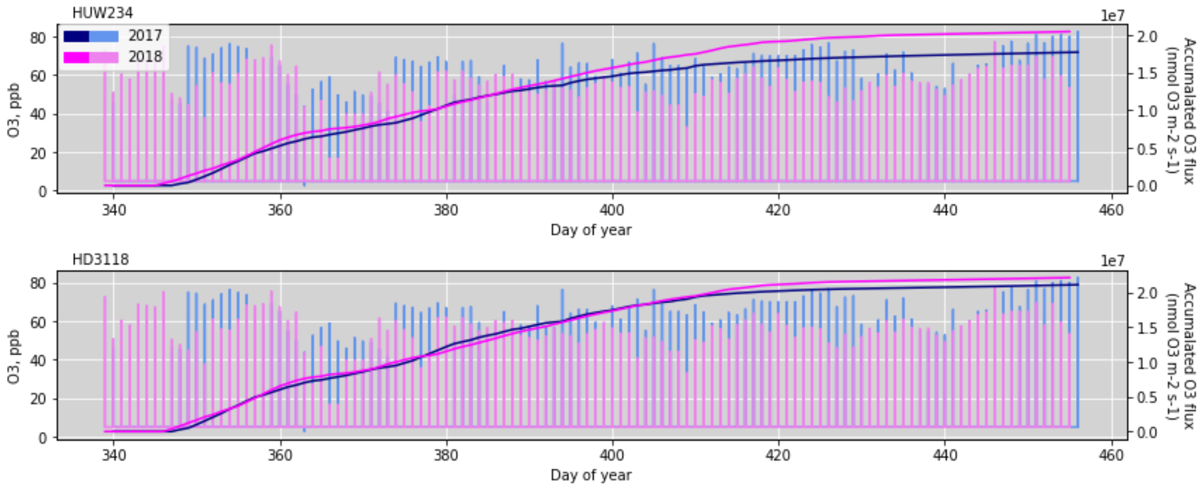

Figure S11: The input O_3 concentrations in parts per billion overlaid with the simulated accumulated stomatal O_3 flux in nmol m^{-2} s^{-1}

Model parameterisation for calibration methods 1 and 2

Both the HUW234 and HD3118 cultivars were ran assuming the number of layers in the canopy was 4, and that there was 1 leaf population (nL=4, nP=1). The HUW234 cultivar parameterisation is given in Table S1, and the HD3118 cultivar parameterisation is given in Table S2.

Table S1: The parameters that were calibrated for (changed from the default parameterisation) in DO_3SE-CropN Model for both calibration methods for the HUW234 cultivar

Process	Parameter description	Calibrated Values		Unit
		Method 1	Method 2	
Phenology	Base temperature (T_b)	7	7	°C

	Optimum temperature (T_o)	25.99	25.99	°C
	Maximum temperature (T_m)	42.637	42.637	°C
	Plant emergence (TT_{emr})	80	80	°C days
	Flag emergence ($TT_{flag,emr}$)	792	792	°C days
	Start anthesis (TT_{astart})	1109	1109	°C days
	Mid-anthesis (TT_{amid})	1181	1181	°C days
	Harvest (TT_{harv})	1668	1668	°C days
Photo-synthesis	Maximum carboxylation capacity at 25 °C ($V_{cmax,25}$)	99.3	99.3	$\mu mol\ CO_2\ m^{-2} s^{-1}$
	Leaf vertical N co-efficient (kN)	0	0	-
	Maximum rate of electron transport at 25 °C ($J_{max,25}$)	138	138	$\mu mol\ CO_2\ m^{-2} s^{-1}$
	Parameter describing the variation in relative stomatal conductance with VPD (VPD_0)	2.95	2.75	kPa
	m (m)	7.4	7.4	-
Respiration	dark respiration (R_{dcoeff})	0.00972	0.00972	-
	growth respiration (R_g)	0.15	0.15	-
DM parameters	Coefficient for determining DM partitioning (α_{root})	16.5	16.64	-
	Coefficient for determining DM partitioning (β_{root})	-21	-20.5	-
	Coefficient for determining DM partitioning (α_{leaf})	20.477	18	-
	Coefficient for determining DM partitioning (β_{leaf})	-24.5	-20	-
	Coefficient for determining DM partitioning (α_{stem})	16.853	15.48	-
	Coefficient for determining DM partitioning (β_{stem})	-17	-14.69	-
	Coefficient determining specific leaf area (Ω)	22.2	22.2	$m^2\ kg^{-1}$
	Fraction of stem carbon in the reserve pool (τ)	0.75	0.75	-
	Fraction of DM in the harvest pool that goes to the grains (rest goes to the ear) (E_g)	0.85	0.85	-
Ozone damage	O_3 long term damage coefficient ($\gamma 3$)	0.0000325	0.0000325	$(\mu mol\ O_3\ m^{-2})^{-1}$
	O_3 long term damage coefficient determining senescence onset ($\gamma 4$)	4.2553	3.1811	-
	O_3 long term damage coefficient determining maturity ($\gamma 5$)	0.944	0.7742	-

	Critical accumulated stomatal O3 flux that determines the onset of leaf senescence (cL_{O_3})	8000	8500	mmol $O_3\, m^{-2}$
N uptake	Pre-anthesis maximum N uptake ($NUP_{pre,max}$)	0.55	0.55	$g\ N\ m^{-2}\ day^{-1}$
	Post-anthesis maximum N uptake ($NUP_{post,max}$)	0.3	0.3	$g\ N\ m^{-2}\ day^{-1}$
Leaf and stem N parameters	Target leaf N concentration ($[N_{leaf,target}]$)	1	1	$g\ N\ m^{-2}$ $leaf\ area$
	Target stem N concentration ($[N_{stem,target}]$)	0.017	0.017	$N\ g^{-1}\ DW$
Grain N parameters	Ratio of N in grain to ear (f_{N,ear_grain})	0.95	0.95	-
	Alpha parameter controlling sigmoid N grain filling function (α_N)	23	23	-
	Beta parameter controlling sigmoid N grain filling function (β_N)	1.2	1.2	-
N re-mobilisation	Gradient of N remobilisation from the leaf under O_3 exposure (m_{leaf})	0.6	0.2	-
	Intercept of N remobilisation from the leaf under O_3 exposure (c_{leaf})	10.89	10.89	-
	Gradient of N remobilisation from the stem under O_3 exposure (m_{stem})	0.0325	0.0325	-
	Intercept of N remobilisation from the stem under O_3 exposure (c_{stem})	0.2293	0.2293	-

Antioxidant processes	Accumulated stomatal O_3 flux above which N is only allocated to antioxidant pool (fst_{end})	45000	45000	mmol $O_3\, m^{-2}$
	Modifier to customise the O_3 effect on antioxidants on the leaf (a_{leaf})	1	1	-
	Modifier to customise the O_3 effect on antioxidants on the stem (a_{stem})	2	2	-

Table S2: The parameters that were calibrated for (changed from the default parameterisation) in DO₃SE-CropN model for both calibration methods for the HD3118 cultivar

Process	Parameter description	Calibrated Values		Unit
		Method 1	Method 2	
Phenology	Base temperature (T_b)	6.992	6.992	°C
	Optimum temperature (T_o)	23	23	°C
	Maximum temperature (T_m)	43	43	°C
	Plant emergence (TT_{emr})	80	80	°C days
	Flag emergence ($TT_{flag,emr}$)	764	764	°C days
	Start anthesis (TT_{astart})	1050	1050	°C days
	Mid-anthesis (TT_{amid})	1093	1093	°C days
	Harvest (TT_{harv})	1450	1450	°C days
Photo-synthesis	Maximum carboxylation capacity at 25 °C ($V_{cmax,25}$)	101.6	101.6	$\mu mol\ CO_2\, m^{-2} s^{-1}$
	Leaf vertical N co-efficient (kN)	0	0.2	-
	Maximum rate of electron transport at 25 °C ($J_{max,25}$)	144	144	$\mu mol\ CO_2\, m^{-2} s^{-1}$
	Parameter describing the variation in relative stomatal conductance with VPD (VPD_0)	3.85	3	kPa
	m (m)	8.1	7.586	-
Respiration	dark respiration (R_{dcoeff})	0.00726	0.00726	-
	growth respiration (R_g)	0.2	0.15	-
DM parameters	Coefficient for determining DM partitioning (α_{root})	16	16	-
	Coefficient for determining DM partitioning (β_{root})	-21.5	-20.5	-
	Coefficient for determining DM partitioning (α_{leaf})	17.5	18	-
	Coefficient for determining DM partitioning (β_{leaf})	-19.921	-20	-

	Coefficient for determining DM partitioning (α_{stem})	15.15	16.6	-
	Coefficient for determining DM partitioning (β_{stem})	-15.714	-16.5	-
	Coefficient determining specific leaf area (Ω)	22.2	22.2	$m^2\ kg^{-1}$
	Fraction of stem carbon in the reserve pool (τ)	0.7	0.7	-
	Fraction of DM in the harvest pool that goes to the grains (rest goes to the ear) (E_g)	0.85	0.85	-
Ozone damage	O_3 long term damage coefficient ($\gamma 3$)	0.00008	0.0000377	$(\mu mol\ O_3\ m^{-2})^{-1}$
	O_3 long term damage coefficient determining senescence onset ($\gamma 4$)	0.9938	6.81	-
	O_3 long term damage coefficient determining maturity ($\gamma 5$)	0.92	1.4	-
	Critical accumulated stomatal O3 flux that determines the onset of leaf senescence (cL_{O_3})	12000	8500	mmol $O_3\ m^{-2}$
N uptake	Pre-anthesis maximum N uptake ($NUP_{pre,max}$)	0.65	0.5	$g\ N\ m^{-2}\ day^{-1}$
	Post-anthesis maximum N uptake ($NUP_{post,max}$)	0.4	0.2	$g\ N\ m^{-2}\ day^{-1}$
Leaf and stem N parameters	Target leaf N concentration ($[N_{leaf,target}]$)	1	1.2	$g\ N\ m^{-2}$ $leaf\ area$
	Target stem N concentration ($[N_{stem,target}]$)	0.025	0.02	$N\ g^{-1}\ DW$
Grain N parameters	Ratio of N in grain to ear (f_{N,ear_grain})	0.95	0.95	-
	Alpha parameter controlling sigmoid N grain filling function (α_N)	23	23	-

	Beta parameter controlling sigmoid N grain filling function (β_N)	1.2	1.2	-
N re-mobilisation	Gradient of N remobilisation from the leaf under O_3 exposure (m_{leaf})	0.2	0.2	-
	Intercept of N remobilisation from the leaf under O_3 exposure (c_{leaf})	10.89	10.89	-
	Gradient of N remobilisation from the stem under O_3 exposure (m_{stem})	0.2293	0.0335	-
	Intercept of N remobilisation from the stem under O_3 exposure (c_{stem})	0.03425	0.15	-
Antioxidant processes	Accumulated stomatal O_3 flux above which N is only allocated to antioxidant pool (fst_{end})	35000	75000	mmol $O_3\, m^{-2}$
	Modifier to customise the O_3 effect on antioxidants on the leaf (a_{leaf})	0.6	1	-
	Modifier to customise the O_3 effect on antioxidants on the stem (a_{stem})	10	2	-

Senescence

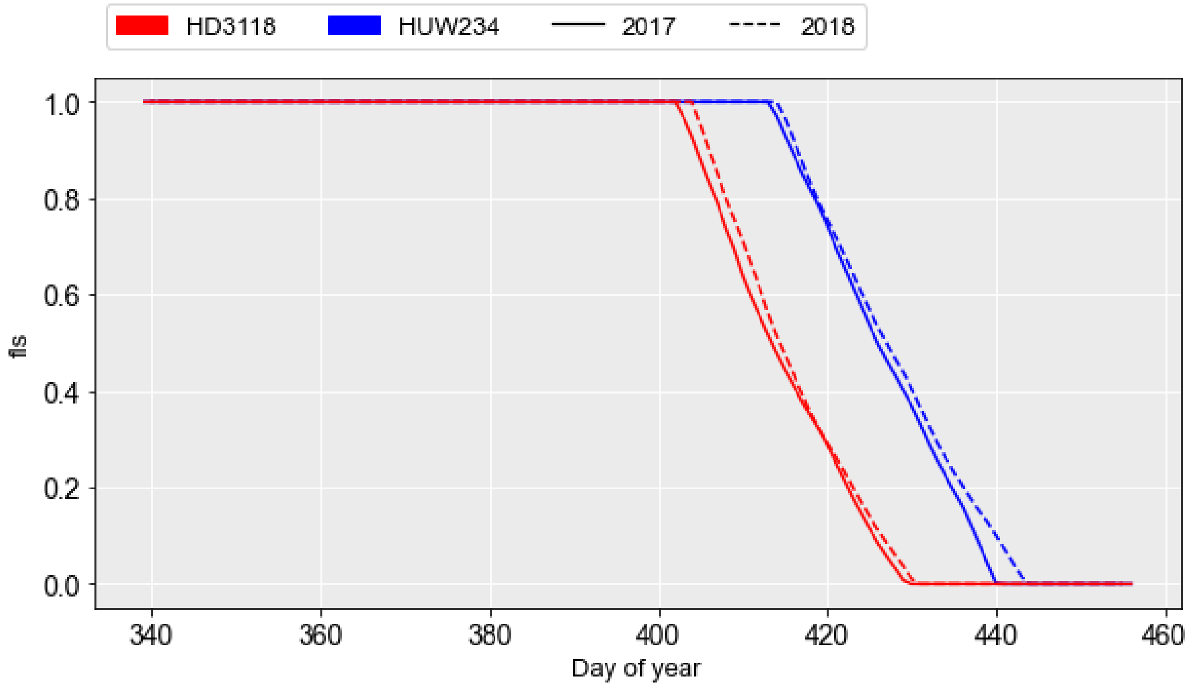

Figure S12: Graph of fls, the factor describing leaf senescence, where 0 is full senescence and 1 is no senescence, for both cultivars and years