Supplement of

Terrestrial Ecosystem Model in R (TEMIR) version 2.0: developing a crop model to simulate the response of maize and soybean to elevated CO_2 and O_3 concentrations

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1. Derivation of ozone damage parameters in the Lombardozzi scheme

Key parameters in the Lombardozzi scheme F_{crit}, $a_{Lombardozzi_An}$, $a_{Lombardozzi_gs}$, $b_{Lombardozzi_An}$, and $b_{Lombardozzi_gs}$ (Equations 5 and 6 in the main text) were derived for each set of ozone exposure experiments. The regression intercepts $b_{Lombardozzi_An}$ and $b_{Lombardozzi_gs}$, which represent the relative A_n and g_s at zero cumulative ozone uptake, respectively, are deviated substantially from unity by default (Lombardozzi et al., 2015). For annual crops that have a well-defined growing season, $b_{Lombardozzi}$ should be set to one to reflect the lack of ozone damage at the beginning of a growing season.

To derive values of F_{crit} and $a_{Lombardozzi}$, trial simulations were conducted with the O_3 damage module enabled but without any modeled ozone damage (i.e., $a_{Lombardozzi} = 0$) to estimate the total effective canopy-level stomatal O_3 uptake during a growing season. Simulations were conducted with F_{crit} values from 0 to 15 nmol O_3 m^{-2} s^{-1} for soybean, and from 0 to 6 nmol O_3 m^{-2} s^{-1} for maize, with an interval of 1 nmol O_3 m^{-2} s^{-1} for both crops. Linear regressions were then constructed for the observed relative reduction in the saturated photosynthetic rate A_{sat} and the observed relative reduction in stomatal conductance against the cumulative effective canopy-level stomatal ozone uptake modeled from each F_{crit}. Typically, the optimal F_{crit} value for the modelling of ozone damage effects on crops is the value that yielded the highest R^2 values in the constructed regressions, following the method, for example, in Pleijel et al. (2004).

A summary of the regression results for soybean data from the SoyFACE experiment (Betzelberger et al., 2012) is shown in Figure S1. Figure S1 (a) shows that a value of F_{crit} = 13 nmol O_3 m^{-2} s^{-1} yields the highest R^2 value for both regressions for the reduction in A_{sat} and g_s against the cumulative ozone uptake, similar to the implemented F_{crit} value of 15 nmol O_3 m^{-2} s^{-1} in the calibrated JULES-crop that also used the same dataset for calibration (Leung et al., 2020). With the modeled cumulative ozone uptake and regression slopes, we estimated the reduction in photosynthetic rate and stomatal conductance under ambient ozone

concentrations relative to a hypothetical O_3-free scenario at each F_{crit} value. Soybean photosynthetic rate and stomatal conductance reduce by 8 – 10 % under ambient ozone concentration (~38 ppb 8-h mean) relative to the O_3-free scenario at F_{crit} = 0 (Figure S1a). With an increasing F_{crit} value, modeled O_3 damage to soybean at ambient ozone concentrations gradually diminishes and the damage is completely nullified at F_{crit} = 9 nmol O_3 m^{-2} s^{-1}. At the statistically optimal F_{crit} value of 13 nmol O_3 m^{-2} s^{-1}, ozone damage is negated even at a target concentration of 70 ppb O_3 (8-h mean: ~55 ppb). To compromise between R^2 values and the modeled ozone damage at lower O_3 concentration levels, we selected 4 nmol O_3 m^{-2} s^{-1} as the F_{crit} value in the model. No field experiment was conducted at very low O_3 concentrations in this dataset to evaluate the damage at ambient O_3 levels relative to O_3-free conditions, therefore it is assumed that the soybean cultivars evaluated in this dataset have the same ozone sensitivity as the soybean cultivars used for the establishment of AOT40 metrics (Mills et al., 2007). With AOT40 values of 3 ppm h in the ambient experiments, a 3 % reduction in crop yield relative to O_3-free conditions is expected, consistent with the 4 % modeled reduction in photosynthetic rate at F_{crit} = 4 nmol O_3 m^{-2} s^{-1}. The mean sensitivity of the relative loss in A_{sat} to the cumulative O_3 uptake across the investigated cultivars is −0.0223 m^2 mmol O_3^{-1} (Figure S1b), and the sensitivity of individual cultivar ranges from −0.0174 to −0.0289 m^2 mmol O_3^{-1}; the mean sensitivity of the relative loss in g_s to the cumulative O_3 uptake is −0.0199 m^2 mmol O_3^{-1}, and the sensitivity for each cultivar ranges from 0 to −0.0300 m^2 mmol O_3^{-1} (Figure S1c).

Summaries of the regression results for maize are shown in Figure S2 and Figure S3. Analysis of the maize data from Peng et al. (2020) and Singh et al. (2023) suggested that F_{crit} values of 6 and 3 nmol O_3 m^{-2} s^{-1} yielded the highest R^2 values for the regression of the relative change in A_{sat} against the cumulative effective stomatal ozone uptake, respectively (Figure S2a). The optimal F_{crit} for the relative change in g_s lies between 3 – 4 nmol O_3 m^{-2} s^{-1} for both sites (Figure S3a). We have decided to implement F_{crit} = 3 nmol O_3 m^{-2} s^{-1} in TEMIR for all maize simulations including O_3. While a value of F_{crit} = 6 nmol O_3 m^{-2} s^{-1} yields the best statistical agreement (R^2 = 0.873) for the A_{sat} observations for data from Peng et al. (2020), the improvement is not substantial over that at F_{crit} = 3 nmol O_3 m^{-2} s^{-1} (R^2 = 0.852). At F_{crit} = 3 nmol O_3 m^{-2} s^{-1}, sensitivities of the reduction in A_{sat} at both sites are similar (Peng: −0.085 ± 0.013 m^2 $mmol^{-1}$ O_3; Singh: −0.124±0.029 m^2 $mmol^{-1}$ O_3). For large-scale evaluations of ozone-induced yield loss where plant-level parameters are difficult to tune for every location, it is preferred to use a single set of damage parameters that can optimally capture the damage. The relationship between the reduction of g_s and the cumulative ozone uptake has greater uncertainty than that of the reduction in A_{sat}. Singh et al. (2023) observed a consistent reduction in g_s with increasing effective stomatal ozone uptake (Fig. S3), regression analysis at F_{crit} = 3 nmol O_3 m^{-2} s^{-1} resulted in a sensitivity parameter of −0.100±0.033 m^2 mmol O_3^{-1}. Peng et al. (2020) observed that g_s decreased with increasing effective stomatal O_3 uptake in the early growing season, but the reduction was less substantial at the later growing season. Regression analysis of the data resulted in an intercept of −0.118, far from the expected value of zero. We therefore propose the value of $a_{Lombardozzi,gs}$ to be −0.05 m^2 mmol O_3^{-1}, which is the slope of the best fit constrained to pass through the origin. The upper limit of $a_{Lombardozzi,gs}$ is −0.10 m^2 mmol O_3^{-1}, which is the sensitivity parameter derived from Singh et al. (2023), whereas the lower limit is zero where g_s does not respond to the cumulative O_3 uptake.

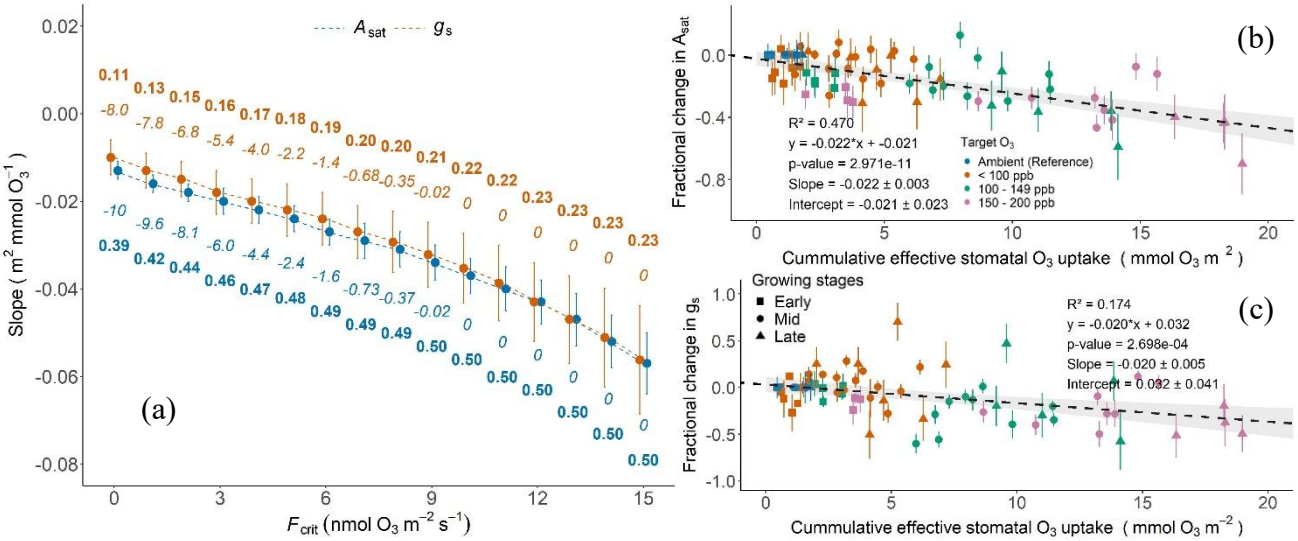


Figure S1. Summary of the regression slope of the relative reduction in A_{sat} and g_s against different stomatal O_3 uptake thresholds F_{crit} in soybean. Numbers in bold are the R^2 value for regression analysis at different F_{crit}. Numbers in italic are the maximum percentage change in the photosynthetic rate or stomatal conductance in the reference experiments at ambient O_3 concentrations, relative to zero O_3 concentration. Data points have been adjusted laterally to enhance visual clarity and readability. (b) and (c) are the regression results of the relative loss of A_{sat} and g_s against the effective stomatal O_3 uptake at F_{crit} = 4 nmol O_3 m^{-2} s^{-1}, respectively.

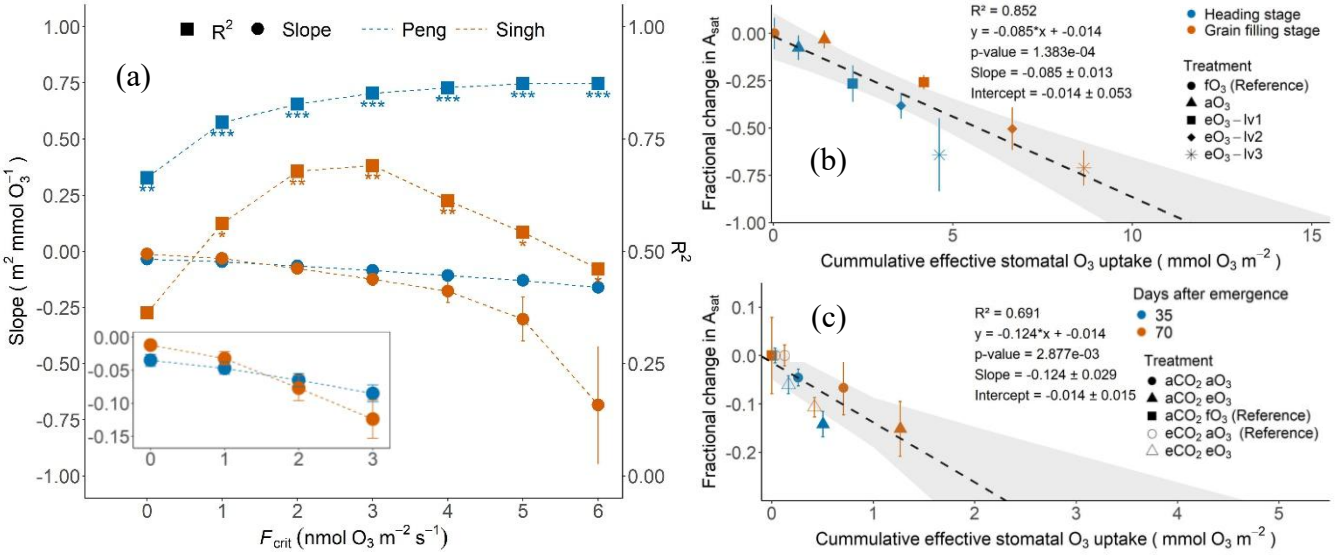


Figure S2. Summary of regression statistics and slopes ($a_{Lombardozzi,An}$) for the relative change in A_{sat} against different stomatal O_3 uptake thresholds F_{crit} in maize (a). Statistical significance is indicated by asterisks: * ($p \leq 0.001$), ** ($p \leq 0.01$), * ($p \leq 0.05$). (b) and (c) are the regression results of the relative loss of A_{sat} against the effective stomatal O_3 uptake at F_{crit} = 3 nmol O_3 m^{-2} s^{-1}, based on the observational data from Peng et al. (2020) and Singh et al. (2023), respectively.**

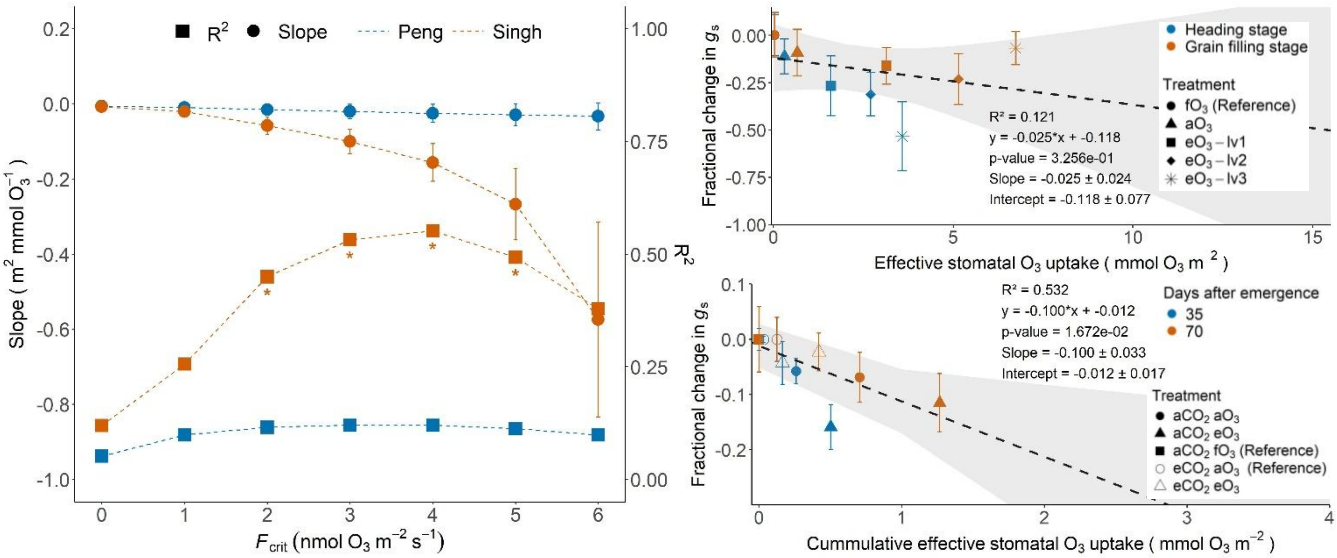


Figure S3. Similar to Figure S2, but showing the regression of the relative decrease in stomatal conductance against the cumulative effective stomatal O_3 uptake thresholds for maize. The regression slopes represent $a_{Lombardozzi,gs}$.

2. Parameters in the crop model

2.1 Derivation of senescence rates of maize and soybean

Additional LAI data other than sites US-Ne2, IN-Hyd, and exposure experiments are used to derive the senescence rate of maize and soybean (Table S1). The timing of the end of the vegetative stage is first determined as the point at which crops reach 90% of their maximum LAI attained during the growing season. Power regressions were fitted using LAI measurements normalized to the maximum growing season LAI against the number of days since the end of the vegetative stage. LAI usually plateaus after the end of the vegetative stage for maize, whereas for soybean, LAI decreases immediately after reaching its maximum value.

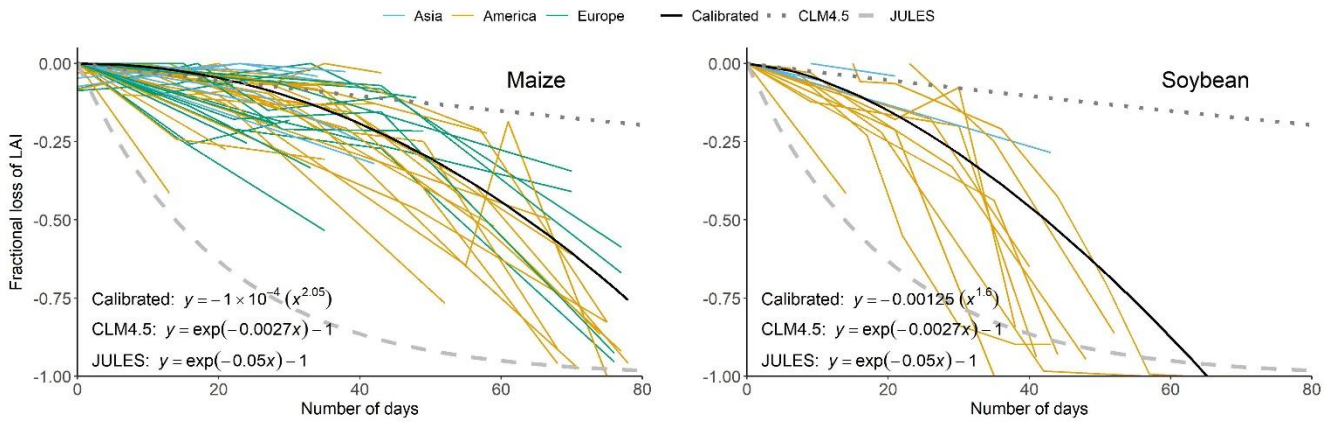


Figure S4. Time series of the fractional loss of normalized LAI (colored lines) after the end of the vegetative stage for maize and soybean. A power regression was fitted to obtain the best fit for each crop; these fits are compared to those simulated with CLM4.5 (dotted line) and JULES-crop (dashed line). Senescence rate parameters (a_{sen}, b_{sen}) used in the model are obtained by taking the derivative of the power regression.

Table S1 LAI data from flux tower sites (except for the CO_2 exposure from Manderscheid et al. 2014) used for the derivation of leaf senescence rate, each growing season has at least three measurements data points.

Sites (abbreviation, if available)	Number of growing seasons	Reference / Data network
Maize		
Mato Grosso, Brazil (BR-CMT)	1	AmeriFLUX
Changwu, China	1	Chinese Ecosystem Research Network
Gucheng, China	4	Chinaflux
Linze, China	1	Chinese Ecosystem Research Network
Klingenberg, Germany (DE-Kli)	1	FLUXNET, ICOS
Borgo Cioffi, Italy (IT-BCi)	8	FLUXNET, ICOS
Braunschweig, Germany	2	Manderscheid et al. 2014
South Great Plains, Oklahoma (US-ARM)	2	AmeriFLUX
Bouldin Island, California (US-Bi2)	3	AmeriFLUX
Mead, Nebraska (US-Ne1, US-Ne2, US-Ne3)	7 (US-Ne1) 4 (US-Ne2 and US-Ne3)	AmeriFLUX, FLUXNET
Rosemount, Minnesota (US-Ro5)	1	AmeriFLUX
Soybean		
Ansai, China	4	Chinese Ecosystem Research Network
Balcarce, Buenos Aires (AR-Bal)	1	AmeriFLUX
Mead, Nebraska (US-Ne2, US-Ne3)	3 for each site	AmeriFLUX, FLUXNET
Rosemount, Minnesota (US-Ro1, US-Ro5)	3 (US-Ro1), 1 (US-Ro5)	AmeriFLUX

Table S2 Parameters for the crop model used in this study.

Variables	Value (maize)	Value (soybean)	Unit	Reference
Phenology				
T_b	8	10	°C	
T_o	30	30	°C	JULES[#]
T_{max}	42	40	°C	
Respiration				
k_{base}	2.53×10^{-6}		gC gN^{-1} s^{-1}	
Q	2		unitless	
CN_{leaf}	10 (before flowering) 65 (after flowering)	25 (before flowering) 65 (after flowering)	unitless	CLM 4.5
CN_{stem}	50 (before flowering) 120 (after flowering)	50 (before flowering) 130 (after flowering)	unitless	
CN_{root}	42	42	unitless	
CN_{repr}	50	60	unitless	
Biomass allocation				
α_{leaf}	13.1	19.2	unitless	
β_{leaf}	−14.1	−14.287	unitless	
α_{stem}	12.1	18.5	unitless	
β_{stem}	−12.1	−13.195	unitless	JULES[#]
α_{root}	13.5	19.8	unitless	
β_{root}	−15.0	−15.47	unitless	
τ	0.12	0.26	unitless	
Leaf senescence				
a_{sen}	-2×10^{-4}	-2×10^{-3}	d^{-1}	This study
b_{sen}	1.05	0.6	unitless	
DVI_{sen}	0.4	1.2	unitless	JULES[#]
Specific leaf area				
SLA_{base}	0.0391	0.0533	m^2 gC^{-1}	JULES[#]
δ	−0.33	0.15	unitless	
f_{CO2}[&]	1 (no available data)	1 at 375 ppm CO_2 0.90±0.05 at 550 ppm CO_2	unitless	Ainsworth et al. (2007)

f_{O3}[&]	1 (no available data)	$1 + 8.2\times10^{-3}(CUO_4)$ See Fig. S5	unitless	Betzelberger et al. (2012)
Crop height				
κ	3.2	1.3	$m^3\ gC^{-1}$	JULES[#] and other flux tower crop height data
λ	0.435	0.41	unitless	

[#] Maize: Williams et al. (2017); Soybean: Leung et al. (2020) [&] Suggested parameterizations, not tested in the simulations.

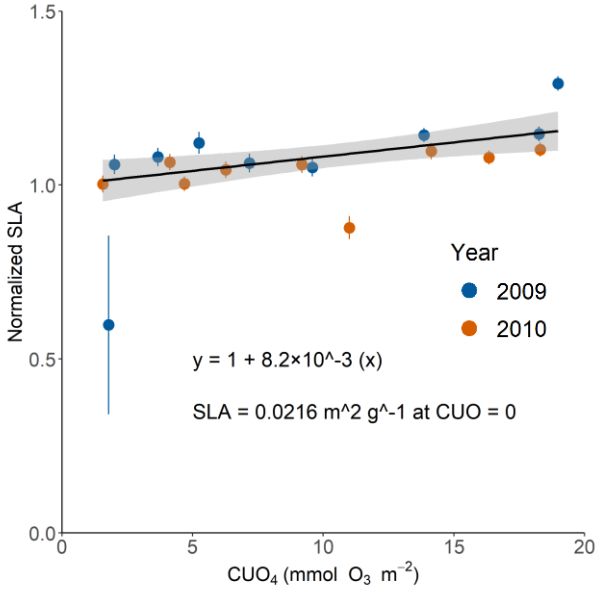


Figure S5. SLA of soybean measured near at the end of a growing season for the experiments conducted in Betzelberger et al. (2012)

Table S3 Site characteristics, NPP:GPP ratio and harvest index of sites US-Ne2, IN-Hyd, and other maize eddy covariance studies

Location	$T_{mean, air}$ (°C)	GPP_{obs} (gC m^{-2})	NPP_{obs} (gC m^{-2})	NPP:GPP	$Harvest_{obs}$ (gC m^{-2})	HI[#]	Reference
Mead, USA	20	1739–1828	964–1028[&]	0.55–0.61	488–538	0.44–0.54	This study Suyker and Verma (2012)
Hyderabad, India	32	791	682[&]	0.86	291	0.43	This study
Wageningen, Netherlands	15	1794	790	0.44	450	0.57	Jans et al. (2010)
Luancheng, China	24	984	540	0.55	310	0.57	Wang et al. (2015)
Weishan, China	23	780	532	0.68	265	0.50	Zhang et al. (2020)

[#] Calculated based on the harvested carbon mass, rather than the whole dry matter mass. [&] Using the maximum attained above-ground biomass as the NPP, as root biomass data are not available. The root:shoot biomass ratio for maize is around 0.05–0.15 based on the data from other eddy covariance sites listed in the table and Ordóñez et al. (2020), which makes the actual NPP:GPP ~10 % larger than the values listed in the table.

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