Author Responses to Reviewer 1 Comments on "Calibrating soybean parameters in JULES5.0 from the US-Ne2/3 FLUXNET sites and the SoyFACE-O3 experiment" by Leung et al., (Manuscript ID: gmd-2020-97-RC1)

Our point-by-point responses are provided below. The referees' comments are *italicized*, texts from the manuscript is in blue and our new/modified text is highlighted in **bold**. The revised manuscript with tracked changes is also included in the linked file below for the Editor's easy reference:

Response to Reviewer #1

We thank the reviewer for the complement and helpful comments. The paper has been revised substantially to address the reviewer's concerns point by point, and all changes are cited and discussed in the responses below.

L47: The authors mentioned "Recently..." but Morgan et al. 2004 is a quite old paper.

Yes, I agree that Morgan et al., 2004 is an old paper. Thank you for suggesting other more recent publications. I have now included them.

Recently the introduction of Free-Air-Concentration-Enrichment (FACE) technology avoids the artefacts from enclosed chambers, and O_3 fumigation was adapted to FACE facilities (Agathokleous et al., 2017; Paoletti et al., 2017).

L147: Better to cite also CLRTAP (2017): <u>https://icpvegetation.ceh.ac.uk/sites/default/files/FinalnewChapter3v4Oct2017_000.pdf</u>

Thanks for the suggestions. I have now updated it here at L148:

To improve these indices, the Stockholm Environment Institute developed the Deposition of Ozone for Stomatal Exchange model (DO₃SE) (**Emberson et al., 2007; ICP Vegetation, 2017**).

L193-194, "... fractional reduction of photosynthesis by O3, F...", "F=1.40", "F=0.25": I suppose not "F" but "a" as you mentioned in lines 168-169. L194, "...equation 1, 2...": I suppose not "equation 1, 2" but "equation 2, 3".

Yes, you are correct. Sorry for the mistakes. Now I have change it in Line 195:

...plant functional types with two different O₃ sensitivities (fractional reduction of photosynthesis by O₃, *F*, *equation 2*, *3*), where a = 1.40 is high sensitivity, and a = 0.25 is lower sensitivity for C3 grass (Sitch, 2007), using monthly average O₃ data and calibration to yield observations.

L221, "Threshold of O3 flux (mmol m-2 s-1)": The unit should be "nmol m-2 s-1".

Yes, you are correct. I have amended it in L222:

We then tuned the O_3 parameterisation of Fractional reduction of photosynthesis by O_3 (sensitivity) and Threshold of O_3 flux (**nmol m-2 s-1**) to match the modelled leaf photosynthesis rate to the observed rate (Figure 2). The tuned parameters are showed in Table 4.

L307: Better to add some brief sentence in order to support your speculation about plant density and leaf area. For example, Jaumer Ricaurte's paper (Ricaurte et al., 2016, Crop Science, vol. 56, pages 2713-2721) would be helpful.

Thanks for the suggestions! This paper is very helpful. I have added a sentence in L310 to support the leaf area results.

Ricaurte et al., (2016) showed that higher sowing density would increase phyllochron in a linear relationship, which results a higher LAI measured that is consistent with our study.

Fig. 2: It is hard to identify symbols (model simulations vs observations). Better to use different colours as you did in the other figures.

Yes, I agree. I have now assigned colours for each symbol in Figure 2.



Figure 2. Net leaf CO_2 assimilation rate for calibrated JULES, simulated using the Leaf Simulator (black crosses) and observations from Betzelberger et al., (2012) (grey circles). X-axis is the daytime 8-hour mean O_3 concentration (ppb)

Table 4: Correct the units. The unit of fractional reduction of photosynthesis should be "mmol-1 m2". Instead, the unit of the threshold of ozone flux should be "nmol m-2 s-1".

Thanks for spotting the error. I have now corrected Table 4.

Author Responses to Reviewer 2 Comments on "Calibrating soybean parameters in JULES5.0 from the US-Ne2/3 FLUXNET sites and the SoyFACE-O3 experiment" by Leung et al., (Manuscript ID: gmd-2020-97-RC1)

Our point-by-point responses are provided below. The referees' comments are *italicized*, the texts from the manuscript are in blue and our new/modified text is highlighted in **bold**. The revised manuscript with tracked changes is also included in the linked file below for the Editor's easy reference:

Response to Reviewer #2

We thank the reviewer for the complement and helpful comments. The paper has been revised accordingly to address the reviewer's concerns point by point, and all changes are cited and discussed in the responses below.

Could crop rotation and irrigation vs. rainfed issues affect the tuning parameters? Introduction and discussion on this are necessary for readers unfamiliar with the sites and the tuning process. In the tuning process, seems like 2002 and 2004 (and 2006 and 2008?) are picked for tuning, why are these years selected? Is it because of data availability or other reasons? Please clarify.

No, crop rotation and irrigation would not affect the tuning. We only simulated the years where soybean is grown. Maize grown in the odd years (2003, 2005 etc.) are not included in our tuning. JULES could simulate irrigation and refed and represent them well. Examples of JULES-crop representing irrigated and rainfed tunings can be found in Williams et al., (2017) Evaluation of JULES-crop performance against site observations of irrigated maize from Mead, Nebraska.

The years 2004, 2006 and 2008 are picked because these are the years which soybeans are grown. I have clarified it in L104

We first tuned the JULES-crop soybean parameterisation at the US-Ne2 and US-Ne3 Mead sites, where three years of soybean physiological and meteorological observations were available, at ambient ozone (Figure 1, steps 1-5). The three years are 2004, 2006 and 2008 which soybeans were grown in Mead, maize were grown in other years.

Section 2.1 description is too short. Could it be extended by two or more sentences with more details in the main manuscript?

Yes, I agree that it is a bit too short. I have now extended it on L123

Step 1 involved using Mead observation to tune the parameters needed by all PFTs in JULES with the crop model switched off. Step 2 is to evaluate the model

performance of GPP using Mead meteorology and LAI. Step 3 tunes the parameters needed by crop only. Step 4 evaluated the JULES-crop run performance with observed carbon pools in leaf, stem, harvest etc. Step 5 demonstrated the full JULES-crop runs at Mead using Mead meteorology and compared the model with observed GPP, aboveground carbon etc. Step 6 tune ozone damage using SoyFACE LiCOR measurements. And finally step 7 evaluates JULES-crop performance using SoyFACE meteorology and compare with observed yield and LAI.

Figure 3, 4 and Section 3 include the major results of this manuscript, which is the evaluation of aboveground carbon and yield against SoyFACE observations and previous model results, and the new, calibrated run underestimates ozone impact significantly at most of the ozone levels. Authors argue that this is due to underestimation of water stress in the model and some testing has been done. Could authors make some assumptions about water stress (like p0=0 mentioned) and include the results in Figure 3 and 4?

Yes, for the p0 value, we used the FAO document 56 (Allen and Pereira, 2006) which used the value p0=0.5 and I showed it in Table 3. I have now showed the results of p0=0 in Supplementary instead to avoid confusion. L262 is now updated

We tested the sensitivity to this choice by re-running this configuration with fsmc_p0=0 which represents water stressed conditions, and this caused a 12% reduction in aboveground carbon (plots show in Supplementary).



Supplementary Figure that shows p0=0 reduce the approximately 12% of the aboveground carbon and yield compared to Figure 3 and 4.

Figure 5, could these figures be condensed into 9 panels or fewer instead of 27? So that three sets of model runs could be compared against each other. Results and discussion around Figure 5 could be easier to comprehend if they are compared side to side.



Yes, you are right. I have condensed them into 9 panels, with each model set in different colours for easier comparison.

Figure 5 Time series of Leaf Area Index (LAI) responses on different target ozone concentration at SoyFACE. Black line is observed LAI from Betzelberger et al., (2012) and the other lines are JULES-crop LAI with different tunings. Blue: calibrated JULES-crop using Mead observations. Green: Osborne 2015 tuning with low sensitivity. Red: Osborne 2015 tuning with high sensitivity to ozone.

Line 138, please include definition of daytime hours. It is 12 hours between 0700 to 1900. It is now changed in L146 **The integral is taken over daytime hours between 0700 to 1900**

Line 183, linear -> linearly

Line 183, photosynthetic rate A, if A will not be used in the manuscript, don't include it. Thanks, it is now changed in L191 ...Given that g_1 and photosynthetic rate are **linearly** related [Cox et al., 1999], g_1 is given by...

Line 189, '(dfp_dcuo_io)' is this used later? If not, don't include it.

It is now changed in L196

Fractional reduction of photosynthesis with the instanteneous uptake of O_3 by leaves (mmol m⁻²) determines the sensitivity of soybean to O_3

Line 173 and line 194, what is this F? is it the same as f in equation 2, 3 and 6. I am confused. Line 193-195 doesn't make sense to me.

Sorry for the confusions. I have change the letter F to be capital letter to make it consistent. Please check L194

 $\boldsymbol{g}_l = \boldsymbol{g}_p \boldsymbol{F} \tag{6}$

Where g_p is the leaf conductance in the absence of O₃ effects. The set of equations (3,5,6) produces a quadratic relationship as a function of *F*, that can be solved analytically (Sitch et al., 2007).

Line 191, should be "… the threshold ozone flux above which ozone would cause damage to …"

Thanks for spotting the mistake. It is now changed in L196

Fractional reduction of photosynthesis with the instanteneous uptake of O_3 by leaves (mmol m⁻²) determines the sensitivity of soybean to O_3 and the PFT-specific O_3 critical level (FO₃ crit) determines the threshold O_3 flux **above** which would cause damage to photosynthesis (Oliver et al., 2018; Sitch et al., 2007).

Line 246, Section 3.1 is not necessary if there is not Sect. 3.2, 3.3, ... and next section should be Section 4, instead of 5. Numbering in Sect. 2 has some issues too, please correct them.

Thanks. I have corrected the numbering in section 2. And I have deleted the title of section 3.1. Please see L254

Results from JULES runs with crop model and ozone damage turned on are showed in Figure 3 and 4.

Simulation names: "Mead tuning", "Osborne 2015 tuning" and "Oseborne 2015 higho3sens tuning" in the figures and in the main text. Could these names be shortened and renamed?

Yes, it is now shortened to "mead", "Osborne 2015", "highO3sen"

Supplementary Figure S1-1, S1-2, S3-2, S3-3 and S3-5, image quality is low (S1-1, low resolution), and presentation is not quite clear. Vertical and diagonal crosses are difficult to differentiate. Caption for Figure S1-2, should be 'Figure S1-1' instead of 'Figure 10'.

Thanks for the comments. We have plotted a higher resolution images in PDF format, I will attached it separately. And the caption for Figure S1-2 is changed in L44

Colours show the cosine for the zenith angle (for legend, see Figure S1-1). Solid black line indicates a = 1.

Figure 4 caption: "... according to Table 4 and Figure 8." There is no Figure 8.

Thanks. Figure 4 caption is now changed in L524

The red line and crosses are the tuned parameters with Mead FLUXNET observation and SoyFACE ozone damage according to **Table 4**.

Figure 3 title unnecessary. Titles and axis labels in other figures are also messy, these need to be fixed for readers to follow.

Sorry about that, I have fixed Figure 3.

Should Figure A2 be included in the supplements instead of the main manuscript? I don't see the necessacity of having appendix and supplements at the same time.

Yes, I agree. I have put the appendix in the supplementary materials.

Calibrating soybean parameters in JULES 5.0 from the US-Ne2/3 FLUXNET sites and the SoyFACE-O₃ experiment

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Abstract. Tropospheric ozone (O_3) is the third most important anthropogenic greenhouse gas. O_3 is detrimental

- 15 to plant productivity, and it has a significant impact on crop yield. Currently, the Joint UK Land Environment Simulator (JULES) land surface model includes a representation of global crops (JULES-crop), but does not have crop-specific O₃ damage parameters, and applies default C3 grass O₃ parameters for soybean that underestimates O₃ damage. Physiological parameters for O₃ damage in soybean in JULES-crop were calibrated against leaf gasexchange measurements from the Soybean Free-Air-Concentration-Enrichment (SoyFACE) with O₃ experiment
- 20 in Illinois, USA. Other plant parameters were calibrated using an extensive array of soybean observations such as crop height, leaf carbon, etc. and meteorological data from FLUXNET sites near Mead, Nebraska, USA. The yield, aboveground carbon and leaf area index (LAI) of soybean from the SoyFACE experiment were used to evaluate the newly calibrated parameters. The result shows good performance for yield, with the modelled yield being within the spread of the SoyFACE observations. Although JULES-crop is able to reproduce observed LAI
- 25 seasonality, its magnitude is underestimated. The newly calibrated version of JULES will be applied regionally and globally in future JULES simulations. This study helps to build a state-of-the-art impact assessment model and contribute to a more complete understanding of the impacts of climate change on food production.

1 Introduction

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Surface ozone (O₃) pollution is one of the major threats to global food security due to the detrimental effects of ozone exposure on crops (Ainsworth et al., 2012; Avnery et al., 2011b; Leung et al., 2020; Long et al., 2005; Tai et al., 2014; Tai andVal Martin, 2017). In the United States alone, crop loss due to tropospheric O₃ costs more than \$5 billion USD annually (Ainsworth et al., 2012; Avnery et al., 2011a; Van Dingenen et al., 2009).

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Soybean is one of the main staple crops for human consumption; it also serves as an important source of animal feed. It is a cheap source of proteins and therefore soybean products are consumed around the world. The impact of O_3 on soybean physiology and growth has been studied extensively (Ainsworth et al., 2012; Betzelberger et al., 2012; Dermody et al., 2008; Morgan et al., 2003). Crop yield losses to tropospheric O_3 have been quantified using

- 40 model projection and experiments. The National Crop Loss Assessment Network and European Open Top Chamber programs have established the air quality guideline, which derived dose-response relationships from comparable experimental data. These campaigns provided critical information such as the O₃ response relationship and estimated yield loss due to O₃ damage that enabled regional projections of O₃ effects on crop yields (Fuhrer, 2009). However, open top chambers modify plant response to O₃ due to the 'chamber effects' which create
- 45 microclimates (Elagöz and Manning, 2005) and environmental differences between the chamber and open air micrometeorology in which yield loss is underestimated (Van Dingenen et al., 2009). Recently the introduction of Free-Air-Concentration-Enrichment (FACE) technology avoids the artefacts from enclosed chambers, and O₃ fumigation was adapted to FACE facilities <u>(Agathokleous et al., 2017; Paoletti et al., 2017)</u>. The application of FACE experiment on crops took place in China (Zhu et al., 2011) and USA, including

50 experiments with soybean at the SoyFACE experiment in Champaign, Illinois (Morgan et al., 2004; Betzelberger et al. 2010; 2012).

Crops are a significant component of the land surface; e.g., croplands and pasturelands represent 12% and 26% of the global terrestrial land, respectively (Van den Hoof et al., 2011). Moreover, the phenology of crops is very
different from that of natural vegetation, and is characterized by high growth, turnover rate, and strong seasonality. It is thus necessary to include a crop-specific parameterization scheme to improve simulations of land surface fluxes and regional climate in agroecosystems (Van den Hoof et al., 2011). The Joint UK Land Environment Simulator with crops (JULES-crop) is a crop parameterisation (Osborne et al., 2015) within the

land surface model, JULES (Best et al., 2011; Clark et al., 2011). Global simulations have been performed with

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JULES-crop for rice, wheat, maize and soybean (Osborne et al., 2015). These four crop types contribute more than 70% of human calorie intake (Ray et al., 2013). JULES-crop includes routines representing growth, development and harvesting of crops driven by the overlying meteorological inputs. In JULES-crop, four new

- 65 prognostic variables have been added: crop development index (DVI), root carbon (Croot), harvest carbon (Charv) and reserve carbon (Cresv). DVI controls the duration of the crop growing season in four distinct stages: sowing, emergence, flowering, and maturity, and it determines when changes in carbon partitioning occur (Osborne and Hooker, 2011). Croot, Charv, and Cresv are the carbon pools for roots, harvested organs (e.g. grains of cereal, fruits, and root) and stem reserves, respectively. Carbon pools for stem and leaves are determined
- from the existing prognostic variables, LAI (Leaf area index) and canopy height. In Osborne et al. (2015), global runs of maize, wheat, soybean and rice were carried out using JULES-crop. Site runs were performed at four FLUXNET sites with soybean-maize rotation: Bondville (US-Bo1), Fermi (US-IB1) and Mead (US-Ne2 and US-Ne3). Simulated yield was compared against country and global FAO crop yields. Osborne et al. (2015) used generic representations for each of the crops in their global study. For the plant parameters that are needed
- 75 outside the crop model such as leaf nitrogen and leaf respiration parameters, these are set to those of the C3 or C4 grass functional types. Osborne et al. (2015) suggested that these parameters could be tuned to be more crop specific to improve fit to observations. These JULES parameters have been calibrated against observations for maize, using data from the Mead FLUXNET sites in Nebraska (Williams et al., 2017). However, to date, these parameters have not been calibrated to soybean data.
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There are many crop models developed by institutions / organisations around the world. Most are designed for application to an individual field up to the regional scale and do not include O₃ impacts on vegetation. (Supplementary Materials Table A1) compares a selection of land surface models which include crop tiles and have the functions to model climate impact on crop productivity. JULES-crop is of particular interest because

- 85 it is a development of the global land surface component JULES of the Met Office numerical weather prediction and climate models, and contains a detailed representation of plant physiological processes at subdiurnal timescales, including consideration of O₃ effects on natural vegetation, thus making it suitable for this study. JULES-Crop has been accepted into the JULES trunk with the intention to be coupled with the Hadley Centre Global Environment Model (HadGEM) in the near future. HadGEM is recognised as one of the best
- 90 performing climate models with smaller errors than typical climate models (Gleckler et al., 2008; Knutti et al., 2013).

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- 95 The calibration of O₃ damage on soybean would allow land surface and crop models to more realistically and reliably simulate present-day and future O₃ damage, and subsequently to quantify its economic impacts. The objective of this study is to calibrate soybean representation for JULES-crop, with a particular focus on the response of soybean to O3 exposure.
- 100 This paper is organised as follows: Section 2 describes the model set-up and observations used for the JULES calibration. Section 3 compares the results from the calibrated JULES runs against independent observations. Section 4 assesses the suitability of the model for modelling soybean under O3 damage and discusses ways of future model improvement.

105 2 Methods

A flowchart demonstrating the calibration and evaluation procedure is given in Figure 1. We first tuned the JULES-crop soybean parameterisation at the US-Ne2 and US-Ne3 Mead sites, where three years of soybean physiological and meteorological observations were available, at ambient ozone (Figure 1, steps 1-5). The three years are 2004, 2006 and 2008 which soybeans were grown in Mead, maize were grown in other years.

Secondly, to calibrate the JULES ozone damage parameters (Figure 1, step 6) we made the assumption that there is a negligible damage to crop yield at ambient background levels of O₃ at both the SoyFACE and Mead sites. This is consistent with Mills et al. (2007), who reviewed over 700 published papers and conference proceedings and found that O3 level of AOT40 over 3 months of 5 ppm-h reduced soybean yield by less than 5%. Then we calibrated specifically the soybean O3 response using leaf gas exchange measurements from soybean grown under elevated O3 concentrations at SoyFACE.

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Finally, we applied JULES-crop newly calibrated for soybean and its O3 sensitivity at the leaf-level and evaluated 120 model performance against observed yield and leaf area index from SoyFACE, taken for the full range of rings and cultivars (Figure 1, step 7).

2.1 Calibration of soybean in the absence of ozone damage, using observations from Mead

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We followed the standard tuning procedure performed on maize by Williams et al., (2017) but applied to soybean (Figure 1, steps1-5). <u>Step 1 involved using Mead observation to tune the parameters needed by all PFTs in JULES with the crop model switched off. Step 2 is to evaluated the model performance of GPP using Mead meteorlogy and LAI. Step 3 tunes the parameters needed by crop only. Step 4 evaluated the JULES-crop run</u>

- 130 performance with observed carbon pools in leaf, stem, harvest etc. Step 5 demonstrated the full JULES-crop runs at Mead using Mead meteorlogy and compared the model with observed GPP, aboveground carbon etc. Step 6 tune ozone damage using SoyFACE LiCOR measurements. And finally step 7 evaluates JULES-crop performance using SoyFACE meteorology and compare with observed yield and LAI. This method is described in detail in the Supplementary Material, and the resulting parameters are given in Table 1-3. These are compared
- 135 to the parameters used in Osborne et al. (2015), which we refer to as the "Osborne 2015 tuning". Note that the parameters in Table 3 in the Osborne 2015 tuning are typical defaults for C3 grass, rather than soybean-specific.

2.2 Calibration of JULES ozone damage parameters

2.2.1 Ozone effects on vegetation (exposure-response)

140 Many studies have shown that the impacts of O₃ are closely related to accumulated exposure above a threshold concentration rather than the mean growing season concentration (Forestry Commission, 2016; Gerosa et al. 2012; Mills et al. 2007). An index of accumulated exposure above a threshold concentration of x ppb (AOTx) has thus been developed as a measure of assessing O₃ pollution effects on vegetation. AOTx is calculated as the summed product of the concentration above the threshold concentration and time (T), with values expressed in ppb h or ppm h. (Mills et al. 2007; Forestry Commission, 2016).

The O₃ exposure index AOT40: Accumulated O₃ exposure over a threshold of 40 parts per billion (Equation 1) has been widely used by crop impact models in the forestry and agriculture industry and was used at SoyFACE.

$A0T40 = \int \max(O_3 - 40ppb, 0.0) dt$ (1)

150 The metric ensures only O₃ concentrations above 40 ppb are included. The integral is taken over daytime hours between 0700 to 1900. AOT40 does not account for the actual uptake of O₃ by plants and how this varies with ontogenetic (life span of the plant) and climatic factors such as temperature, irradiance, vapour pressure deficit, and/or soil moisture (Ashmore, 2005; Fuhrer et al. 1997).

- 155 There is a drawback of the cumulative O₃ exposure indices (Pleijel et al. 2000), which assume an instantaneously fixed threshold flux below which there is no effect of O3, which may not be realistic. Also in nature, the threshold value is unlikely to be constant (Ashmore, 2005) since the capacity of detoxification of O₃ varies with climate and plant species. To improve these indices, the Stockholm Environment Institute developed the Deposition of Ozone for Stomatal Exchange model (DO3SE) (Emberson et al., 2007; ICP Vegetation, 2017). DO3SE was developed to
- 160 estimate the risk of O3 damage to European vegetation and is capable of providing O3 flux estimation by evaluating the soil water deficits and their influence on stomatal conductance which affect plant O3 uptake. Phyto-toxic O3 dose (POD) above a stomatal threshold over a growing season (the accumulated stomatal flux above threshold Y) PODy can differentiate species sensitivity to rising background concentration, while AOT40 can only incorporate the effect of rising global background O3 above the threshold 40ppb. This difference means AOT40 metric is less
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2.2.2 Description of ozone response scheme in JULES

The current O3 scheme in JULES uses a dose-response approach to model O3 damage (Sitch et al., 2007; Clark et al., 2011). It uses the O₃ concentration in the atmosphere to modify net photosynthesis A_p by an O₃ uptake factor

sensitive to O₃ peaks, and stomatal flux based metric (e.g. PODy and DO3SE) perform better on O₃ damage estimation in general (Büker et al., 2012; Dentener, F., Keating, T., and Akimoto, 2010; Pleijel et al., 2007).

	<u>F</u> :		Deleted: f
	$A = A_p \frac{E_r}{2} (2)$		Deleted: f
	where \sqrt{r} represents the fractional reduction of plant production:	(Deleted: f
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	$F_{a}=1-aUO_{>FO3crit}$ (3)	< (Formatted: Font: Italic
	It assumes that O ₃ suppresses the potential net leaf photosynthesis in proportion to the O ₃ flux through stomata	(Deleted: f
	above a specified critical threshold (Clark et al., 2011).		
180	$UO_{>F O3crit}$ is the instantaneous leaf uptake of O ₃ over a plant functional type specific threshold (F_{O3crit}) (nmol m ⁻² s ⁻¹) and the plant type specific parameter <i>a</i> is the fractional reduction of photosynthesis with O ₃ uptake		Formatted: Subscript
	by leaves (Clark et al., 2011; Sitch et al., 2007).		

$UO_{>FO3crit} = \max[(F_{O3}-F_{O3crit}), 0.0]$ (4)

From equations 3 & 4, *F* depends on the O₃ uptake rate by stomata (F_{O3}) over a critical (plant functional type specific) threshold for damage. It uses an analogy of Ohm's law, the O₃ flux through stomata, F_{O3} (nmol O₃ m⁻² s⁻¹), is given by,

$$F_{03} = \frac{[O_3]}{R_a + \left[\frac{\kappa_{03}}{gl}\right]}$$
(5)

195 where $[O_3]$ is the molar concentration of O₃ at reference level (nmol m⁻³), R_a is the combined aerodynamic and boundary layer resistance between leaf surface and reference level (s m⁻¹). g_1 is the leaf conductance for H₂O (m s⁻¹), and $\kappa_{O3} = 1.67$ is the ratio of leaf resistance for O₃ to leaf resistance for water vapour [Sitch et al., 2007]. The uptake flux is dependent on the stomatal conductance, which is reliant on the photosynthetic rate in JULES. Given that g_1 and photosynthetic rate are linearly related [Cox et al., 1999], g_1 is given by, 200 $g_1 = g_p F$ (6)

Where g_p is the leaf conductance in the absence of O₃ effects. The set of equations (3,5,6) produces a quadratic relationship as a function of F_{\bullet} that can be solved analytically (Sitch et al., 2007).

- Fractional reduction of photosynthesis with the instanteneous uptake of O₃ by leaves (mmol m²) determines the sensitivity of soybean to O₃ and the PFT-specific O₃ critical level (FO₃ crit) determines the threshold O₃ flux above which would cause damage to photosynthesis (Oliver et al., 2018; Sitch et al., 2007). The higher the sensitivity of plants to O₃ the lower photosynthesis the plant has at a given constant critical threshold. Sitch et al. (2007) configured plant functional types with two different O₃ sensitivities (fractional reduction of photosynthesis
 by O₃, *F*, equation 2, 3), where a = 1.40 is high sensitivity, and a = 0.25 is lower sensitivity for C3 grass (Sitch,
- 2007), using monthly average O₃ data and calibration to yield observations.

2.2.3 Calibrating the ozone effects on crop leaf photosynthesis in JULES using SoyFACE

The SoyFACE experiment in Illinois allows controlled CO₂ or O₃ enrichment across large plots within a soybean field without an enclosure. SoyFACE O₃ fumigation typically began after the emergence of soybean, and the plots Deleted: A

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- 220 were fumigated with O₃ for 8–9 hours daily except when leaves were wet. In 2009 and 2010, soybeans were exposed to nine different concentrations of O₃ ranging from the ambient level to a target level of 200 ppb (Figure A2). The fumigation ended when soybean was mature.
- Plant damage from O₃ is cumulative and the target concentration for the experiment was not always met (e.g., when wind speeds are low, during rain or when O₃ generators or analyzers are down). Therefore, the 8-hour mean and the AOT40 index (Accumulated Ozone exposure above the Threshold of 40 ppb) were used for the analysis in SoyFACE instead of using the target O₃ concentration. The planting dates were June 6, 2009 (Day 159) and May 27, 2010 (Day 157). Fumigation began on June 29, 2009 (Day 179 260) and June 6, 2010 (Day 167 271) and harvest occurred on October 20, 2009 (Day 293) and September 20, 2010 (Day 273). O₃ concentrations
 measured at SoyFACE fluctuated greatly, as they were strongly influenced by weather conditions, especially by wind speed. The magnitude of O₃ concentration fluctuations in the high targeted concentration was greater than the low concentration (Figure A2). On some days of the year when the fumigation was off, very low O₃ concentrations were recorded for all target rings.
- 235 To calibrate the O₃ parameters for soybean in JULES-crop, we used midday photosynthetic gas-exchange measurements from Betzelberger et al. (2012). These were taken at four stages during the growing season, from seven soybean cultivars growing at 9 different O₃ concentrations, using open gas exchange systems (LI-6400 and LI-6400-40). These observations were used in conjunction with the daytime 8-hour mean O₃ concentration measurements and the parameters calibrated at the Mead site to drive the Leaf Simulator computer package, which reproduces the calculation of leaf photosynthesis within JULES. We then tuned the O₃ parameterisation of
- Fractional reduction of photosynthesis by O₃ (sensitivity) and Threshold of O₃ flux (nmol m-2 s-1) to match the modelled leaf photosynthesis rate to the observed rate (Figure 2). The tuned parameters are showed in Table 4.

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2.3 Model configuration for the JULES-crop SoyFACE runs

The meteorological forcing data measured at Champaign, Illinois in 2009 (Ainsworth et al., 2010) were used to drive the JULES-crop model. The downward longwave radiation and diffuse radiation data from NOAA at Bondville site (SURFRAD) were used as SoyFACE does not have these variables available. The driving data were

repeatedly applied (recycled 25 times) to spin up the model from an arbitrary starting point with soil temperature initially set to 278 K and soil moisture to 75% of saturation. A single crop type was modelled – soybean – using a single plant tile. Observed CO₂ (NOAA) and 8-hour mean observed O₃ concentrations from the SoyFACE rings (averaged over a month) were used as the driving data of the model since natural O₃ is produced around 8 hours in daytime and it is a typical temporal resolution for O₃ fumigation. The soil ancillary parameters used in SoyFACE were extracted from the global dataset of soil ancillary from the HadGEM2-ES model (a coupled Earth System Model that was used by the Met Office Hadley Centre for the CMIP5). Observed ambient O₃ were used

as the control. The new parameters for soybean were used, which we calibrated to observations from the Mead FLUXNET sites as described in the supplementary material. The exception is the initial carbon: since the row

spacing at the SoyFACE experiment is half that used at the Mead sites, we doubled the initial carbon for SoyFACE compared to Mead. The resulting model yield, above ground carbon and LAI was compared to the SoyFACE

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observations.

265 3 Results and Discussion

Results from JULES runs with crop model and ozone damage turned on are showed in Figure 3 and 4. Figure 3 4 shows the evaluation of the soybean aboveground biomass carbon for different O₃ exposure levels (AOT40) using the O₃ damage parameters in Table 4. The model aboveground carbon (solid lines) are compared to the line fitted in Betzelberger et al 2012 to their aboveground carbon observations. The run with the newly-calibrated 270 parameters overestimated the carbon at ambient ozone levels. One contributing factor could be that water stress is underestimated in the new configuration, since it was not possible to evaluate the response to soil water availability using the Mead site data, so we instead derived a value for fsmc p0 (parameterise in the calculation of the threshold for water stress, see Table 3) from literature. We tested the sensitivity to this choice by re-running this configuration with fsmc p0=0 which represents water stressed conditions, and this caused a 12% reduction 275 in aboveground carbon (plots show in Supplementary). In addition, the representation of the soil properties in the JULES SoyFACE run could be improved by calibration to site measurements. In contrast, the "Osborne 2015 tuning" intersects the line fitted to observed aboveground carbon at zero ozone concentration (partially because of higher water stress), but then shows a sharp decrease from zero to ambient levels, which is not realistic. Note that no observations were taken for below-ambient ozone concentrations at SoyFACE, so this section of the fitted 280 line is an extrapolation. The slope of the aboveground carbon response to increasing ozone concentrations is similar for all three runs, and compares very well to the Betzelberger et al 2012 fitted line.

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The yield-O₃ response curve in Figure 4 show that new parametrisation slightly overestimates yield in the ambient SoyFACE ring, compared to the spread of SoyFACE yield observations from Betzelberger et al 2012. The 'Osborne 2015 tuning' with high ozone sensitivity is within the spread of measured yield in ambient conditions,
but note that the modelled yield has decreased sharply from zero ozone concentration to ambient levels, which is undesirable. The magnitude of the gradient of yield against AOT40 for all three model configurations is within the spread of the observations. However, the slope is underestimated for the new, calibrated run and overestimated for the 'Osborne 2015 tuning', especially for the range from ambient to 40 ppm h. Recall that ozone concentration modifies net leaf CO₂ assimilation rate in JULES, and that the model parameters governing this process (*Fo3crit, a*) are calibrated directly to net leaf CO₂ assimilation rate observations from SoyFACE in our new configuration (Section 2). Reductions in the modelled net leaf CO₂ assimilation rate lead to the reductions in model aboveground biomass, yield and LAI which we show in this section. However, Betzelberger et al 2012 also reported additional impacts of ozone damage, such as changes in leaf absorptance and specific leaf mass, that are not represented in JULES, and therefore our tuning does not account for them. In contrast, the values of *Fo3crit* and *a* in the high

- 300 and low sensitivity versions of the 'Osborne 2015 tuning' simulations (table 4) were calibrated in Sitch et al 2007 to yield observations. Therefore, they can be seen as 'effective' parameters in these configurations, since they incorporate the effect of the ozone damage processes that are not explicitly represented in JULES.
- 305 Note that we plot AOT40 on the x-axis for illustrative purposes only, to be comparable with results presented in Betzelberger et al 2012 - AOT40 was not used in the JULES run. An alternative would be to plot ring number or ring target concentration. Ideally, we would plot the x-axis with the metric Phytotoxic Ozone Dose (POD) for JULES and observed data, which account the dosage of O₃ that get into the stomata of soybean, but is beyond the scope of the present study.

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Figure 5 compares the model and observed LAI at SoyFACE for different O₃ concentrations. JULES was able to reproduce LAI seasonality; however, it underestimated the amplitude. The maximum LAI for calibrated JULES peaked around day 240 in September and observations peaked at DOY 220~230. The peak LAI in the model runs was less than half the observed LAI in all cases. While the Mead model runs also showed a slight underestimation

315 of peak LAI compared to observation (Supplementary Materials), the majority of the underestimation of the modelled SoyFACE LAI is due to a difference between the observed relationships between peak LAI and yield at the Mead and SoyFACE sites. At both sites, observed maximum yield increases with observed peak LAI. However, for similar observed yields, the observed SoyFACE yield tends to be higher than the observed Mead LAI. Given that our calibration is based on Mead observations, it is therefore not surprising that our model runs at SoyFACE underestimate peak LAI compared to the SoyFACE observations.

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A contributing factor to the different relationship between observed peak LAI and observed yield at SoyFACE compared to Mead could be the different methods used to measure LAI at the Mead sites (which this parameter set was tuned against) and at SoyFACE. At Mead, destructive measurements were taken, whereas at SoyFACE, LAI was measured indirectly, using radiation attenuation through the canopy.

Another plausible contributing factor for the different relationship between observed peak LAI and observed yield at SoyFACE compared to Mead is the row density of the soybean. The SoyFACE row spacing was half that of Mead so, as described above, we set the initial carbon to twice that observed at Mead. The denser planting allowed soybean at SoyFACE to reach higher LAI earlier in the growing season. If this also resulted in thinner leaves at the beginning of the season than with the Mead row spacing, then this could explain the difference in the peak LAI to yield relationship between the two sites. <u>Ricaurte et al., (2016) showed that higher sowing density would increase phyllochron in a linear relationship, which results a higher LAI measured that is consistent with our study.</u>
JULES also does not account for leaf age on leaf assimilation rate - in reality a lower leaf assimilation is observed

335 in the late season associated with leaf aging, and it is plausible that this could also be affected by row spacing.

Figure 5 also demonstrates that model LAI responds more to ozone concentrations than the observed LAI. One contributing factor is the observed decrease in specific leaf area at SoyFACE in increased ozone (Betzelberger et al 2012). As mentioned above, this process is not captured by JULES. This issue is particularly pronounced in the

340 Osborne 2015 tuning runs, where the modelled LAI in the ring with target 200ppb is roughly a third of the peak LAI in the ambient ring.

5 Conclusions

345 Climate change and air pollution are a great threat to food production. JULES-crop has been developed to represent crops in the land surface model and allow us to estimate the future climate and air pollution impact to crops. The O₃ impact on crops could be quantified with an improved parameterization to the existing O₃ damage scheme for C3 plants. The default soybean biochemical and respiratory parameters in JULES were based on C3 grass parameters. Characteristics of soybean are more similar to a shrub than grass, therefore parameter calibration is needed to improve the performance of soybean in JULES-crop.

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In this paper, the parameters needed to describe soybean in JULES-crop were first revised against observations from the Mead FLUXNET sites to ensure that the crop, biochemical and respiratory parameters explicitly represented soybean. Compared with observations from these sites showed that GPP and LAI were well

- 355 represented for irrigated soybean at Mead. The O₃ damage parameterisation was subsequently calibrated against leaf gas exchange observations from the Soybean Free-Air-Concentration-Enrichment (FACE) experiment for the O₃ damage, by tuning the sensitivity and critical threshold of O₃ damage. On the whole, JULES-Crop reproduces the observed negative correlation between yield and O₃ exposure. It also reproduced the negative impacts of ozone on LAI, and the seasonality of phenology, although the simulated LAI was underestimated at SoyFACE. This
- 360 method of calibrating soybean could be replicated for other crops once data become available and would contribute to more accurate parameters for crop models. The calibration will be applied to a regional and transient run and eventually the newly calibrated JULES-crop for soybean and its sensitivity to O₃ damage, coupled within an Earth System Model.

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Code availability. This study uses JULES version 5.0 releases. The code and configuration for the SoyFACE runs can be downloaded via the Met Office Science Repository Service (MOSRS) at <u>https://code.metoffice.gov.uk/trac/roses-u/browser/a/r/8/6/6/trunk</u> (JULES Collaboration, 2018)(registration required) and are freely available subject to completion of a software licence. The Leaf Simulator can be downloaded from https://code.metoffice.gov.uk/trac/utils (Williams et al., 2018) (login required).

Data availability. Unless otherwise noted, all site observations discussed in this paper were obtained from the

375 Site Information pages of the AmeriFlux website hosted by Oak Ridge National Laboratory (<u>http://fluxnet.fluxdata.org/</u>,(AmeriFlux collaboration, 2018)) or by personal communication with the Mead sites Research Technologist. The longwave radiation, diffuse radiation and air pressure from Bondville, Illinois site is obtained by the SURFRAD (Surface radiation) network from <u>ftp://aftp.cmdl.noaa.gov/data/radiation/surfrad/Bondville_IL/</u>. The SoyFACE data used for the run are available

380 on MOSRS at:

https://code.metoffice.gov.uk/trac/roses-u/browser/a/r/8/6/6/trunk/driving_data https://code.metoffice.gov.uk/trac/roses-u/browser/a/r/8/6/6/trunk/bin/SoyFACE_gas_exchange_data_2009.csv https://code.metoffice.gov.uk/trac/roses-u/browser/a/r/8/6/6/trunk/ancil_data Accessing the MOSRS requires registration, but once you access into the system, there's no information about

385 who is downloading or viewing which pages.

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525 Figure 1. Flowchart of tuning the parameters and calibrating the model





Figure 2. Net leaf CO₂ assimilation rate for calibrated JULES, simulated using the Leaf Simulator (black crosses) and observations from Betzelberger et al., (2012) (grey circles). X-axis is the daytime 8-hour mean O₃ concentration (ppb) .

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Figure 3. Aboveground carbon biomass of soybean at harvest stage for calibrated Joint UK Land Environment Simulator with Crop module turned on (JULES-crop) using the Mead soybean tuning (red), Osborne et al. (2015) standard parameters with Sitch et al. (2007) low ozone sensitivity (blue), high ozone sensitivity (green) and observation from SoyFACE from Betzelberger et al. 2012.





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Figure 4 Black dashed line is the line of best fit from SoyFACE observation and the blue and green lines with crosses are the modelled output for each ozone concentration using the Osborne et al 2015 tuning with Sitch et al 2007 low and high sensitivity, respectively. The red line and crosses are the tuned parameters with Mead FLUXNET observation and SoyFACE ozone damage according to Table 4,

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Figure 5 Time series of Leaf Area Index (LAI) responses on different target ozone concentration at SoyFACE. Black line is observed LAI from Betzelberger et al., (2012) and the <u>other lines are JULES-crop LAL with</u> <u>different tunings. Blue</u>: calibrated JULES-crop using Mead observations. <u>Green</u>: Osborne 2015 tuning with low sensitivity. <u>Red</u>: Osborne 2015 tuning with high sensitivity to ozone.

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 Table 1. JULES modules switches, which F (False) means turned off and T (True) means turned on. Asterisk indicates parameter was hard-wired and the description of the parameters at the bottom

	Osborne et	al., This study	Discussion
	(2015)		
can_rad_mod	5 (6 was	not 6	Recommended option for layered canopy in version 4.6
	available)		
l_irrig_dmd	F	Т	Irrigation on
irr_crop	-	0	
l_trait_phys	F	F	
l_scale_resp_pm	F	Т	
l_leaf_n_resp_fix	F	-	Bug fix, affects can_rad_mod=5 but not can_rad_mod=6
l_prescsow	Т	Т	Sowing dates available

Parameters	Description
Canopy radiation	Number 6 is Multi-layer approach for radiation interception following the 2-stream approach of
model	Sellers et al. (1992). This approach takes into account leaf angle distribution, zenith angle, and
	differentiates absorption of direct and diffuse radiation. it has a decline of leaf N with canopy
	height. Additionally includes inhibition of leaf respiration in the light. including:
	Sunfleck penetration though the canopy.
	Division of sunlit and shaded leaves within each canopy level.
	A modified version of inhibition of leaf respiration in the light.
	exponential decline of leaf N with canopy height proportional to LAI, following Beer's law.
L_irrid_dmd	Switch controlling the implementation of irrigation demand code.
Irr_crop	Irrigation season (i.e. season in which crops might be growing on the gridbox) lasts the entire
	year.
l_trait_phys	Switch for using trait-based physiology. Vcmax is calculated based on parameters nl0 (kgN kgC-
	1) and neff.
l_scale_resp_pm	Soil moisture stress reduces leaf, root, and stem maintenance respiration.
l_leaf_n_resp_fix	Switch for bug fix for leaf nitrogen content used in the calculation of plant maintenance
	respiration.
l_prescsow	Sowing dates prescribed

Table 2. Parameter values in JULES-crop that are used to represent soybean. Asterisk indicates parameter was hard-wired.

		Osborne et al., (2015)	This study	Discussion
Tb	Base temperature (K)	278.15	278.15	Kept at Osborne et al., (2015) value
To	Optimum temperature(K)	313.15	313.15	Kept at Osborne et al., (2015) value
Tm	Maximum temp (K)	300.15	300.15	Kept at Osborne et al., (2015) value
Psen	Sensitivity of development rate to photoperiod (hours-1)	0.0	0.0	Kept at Osborne et al., (2015) value
Pcrit	Critical photoperiod (hours)	-	-	Not used when $P_{sen} = 0$
<i>r</i> dir	coefficient determining relative growth of roots vertically and horizontally	0.0	0.0	Kept at Osborne et al., (2015) value
αroot	coefficient of partitioning to root	20.0	19.8	Supplementary Material 1.4.1
astem	coefficient of partitioning to stem	18.5	18.5	Supplementary Material 1.4.1
αleaf	coefficient of partitioning to leaf	19.5	19.2	Supplementary Material 1.4.1
β root	coefficient of partitioning to root	-16.5	-15.47	Supplementary Material 1.4.1
βstem	coefficient of partitioning to stem	-14.5	-13.195	Supplementary Material 1.4.1
β leaf	coefficient of partitioning to leaf	-15.0	-14.287	Supplementary Material 1.4.1
γ	coefficient of specific leaf area $(m^2 kg^{-1})$	25.9	24.0	Supplementary Material 1.4.3
δ	coefficient of specific leaf area $(m^2 kg^{-1})$	-0.1451	0.15	Supplementary Material 1.4.3
τ	Remobilisation factor, fraction of stem growth partitioned to RESERVEC	0.18	0.26	Supplementary Material 1.4.3
<i>fC</i> ,root	Carbon fraction for dry root	0.5	0.47	Supplementary Material 1.4.4
<i>fC</i> ,stem	Carbon fraction for dry stem	0.5	0.49	Supplementary Material 1.4.4
fC, leaf	Carbon fraction for dry leaf	0.5	0.46	Supplementary Material 1.4.4

<i>fC</i> ,harv	r Carbon fraction for harvest	0.5	0.53	Supplementary Material 1.4.4
κ	Allometric coefficient relating	1.6	1.9	Supplementary Material 1.4.2
	STEMC to CANHT			
λ	Allometric coefficient relating	0.4	0.47	Supplementary Material 1.4.2
	STEMC to CANHT			
μ	Allometric coefficient for	0.05*	5.0	Supplementary Material 1.4.2
	calculation of senescence			
ν	Allometric coefficient for	0.0*	6.0	Supplementary Material 1.4.2
	calculation of senescence			
DVIsen	DVI at which leaf senescence	1.5*	1.25	Supplementary Material 1.5
	begins			
Cinit	Carbon in crop at emergence in	0.01*	3.5E-3	Supplementary Material 1.4.5
	kgC/m2.		(Mead),	
			7.0E-	
			3(SoyFACE)	
DVIinit	DVI at which the crop carbon is	0.0*	0.2	Supplementary Material 1.4.5
	set to initial carbon			
Tmort	Soil temperature (second level) a	t_bse_io*	263.15	Section 2.3
	which to kill crop if DVI>1			
fyield	Fraction of the harvest carbon	1.0*	0.74	Section 2.3
	pool converted to yield carbon			

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		Osborne et al (2015)	., This study	Discussion
<i>c</i> 3	c3_io	1	1	Soybean is a C3 plant.
dr	rootd_ft_io	0.5	0.5	Not important in irrigated runs, so could not be tuned using US-Ne2 data. Kept at Osborne et al, (2015) value
dqcrit	dq_crit_io	0.1	0.1	Kept at Osborne et al., (2015) value
f_d	fd_io	0.015	0.008	Supplementary Material 1.4.6
f0	f0_io	0.9	0.9	Kept at Osborne et al., (2015) value
neff	neff_io	8.0×10^{-4}	12.0×10^{-4}	Table 1
$n_{l(0)}$	nl0_io	0.073	0.1	Table 1
Tlow	tlow_io	0.0	0.0	Kept at Osborne et al., (2015) value
Tupp	tupp_io	36.0	36.0	Kept at Osborne et al., (2015) value
kn	kn_io	0.78	-	Default for C3 grass for can_rad_mod5.
knl	knl_io	-	0.2	Default for C3 grass for can_rad_mod6.
Q10,1eaf	q10_leaf_io	2.0	2.0	Kept at Osborne et al., (2015) value
μrl	nr_nl_io	1.0	0.390	Supplementary Material S1-3
μ_{Sl}	ns_nl_io	1.0	0.51	Supplementary Material S1-3
rg	r_grow_io	0.25	0.32	Supplementary Material 1.4.6
	orient_io	0	0	Kept at Osborne et al., (2015) value
α	alpha_io	0.12	0.12	Kept at Osborne et al., (2015) value
ωPAR	omega_io	0.15	0.15	Kept at Osborne et al., (2015) value
αPAR	alpar_io	0.1	0.1	Kept at Osborne et al., (2015) value
	fsmc_mod_io	0	0	Not important in irrigated runs, so could not be tuned using US-Ne2 data. Kept at Osborne et al (2015) value.
	fsmc_p0_io	0.0	0.5	FAO document 56 (Allen andPereira, 2006)
а	can_struct_a_io	1.0	1.0	Kept at Osborne et al., (2015) value

 Table 3. JULES plant functional type parameters extended to represent soybean. Asterisk indicates parameter

 was hard-wired.

Table 4. Summary of ozone parameter configurations employed in JULES-crop for the default Osborne et al.,

 (2015) value and the tuned as calibrated to SoyFACE leaf gas-exchange measurements (note that these have

 been calibrated to daytime 8-hour concentrations and therefore will be different to parameters calibrated to

 monthly 24hour means)

	Fractional reduction of photosynthesis	Threshold of ozone flux
JULES ozone damage Parameters	by O ₃ (sensitivity) (mmol $\frac{1}{2}$ m ²)	(<u>n</u> mol m ⁻² s ⁻¹)
	(dfp_dcuo_io)	(fl_o3_ct_io)
Tuned value	0.5	15.0
Osborne et al 2015 (High sensitivity)	5.0	1.4
Osborne et al 2015 (Low sensitivity)	5.0	0.25

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