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# **Modelling inclusion, testing and benchmarking of the impacts of ozone pollution on crop yields at regional level**

**Module development and testing and benchmarking with the WOFOST generic crop model**

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JRC103907

EUR 28395 EN

PDF ISBN 978-92-79-64945-5 ISSN 1831-9424 doi:10.2788/68501

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Luxembourg: Publications Office of the European Union, 2016

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How to cite this report: G. Cappelli, R. Confalonieri, M. Van Den Berg, F. Dentener; *Modelling inclusion, testing and benchmarking of the impacts of ozone pollution on crop yields at regional level*; EUR 28395 EN, Luxembourg: Publications Office of the European Union, 2016, doi:10.2788/68501

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## Abstract

The WOFOST crop model -as implemented in the BioMA modelling framework- was extended with algorithms to account for the effects of ground-level ozone on crop growth and yield.

The additional algorithms implemented concern:

- Effect of water stress on stomatal conductance
- Reduction of carboxylation rate of Rubisco
- Ability of plants to partly recover from ozone damage
- Acceleration of leaf senescence due to O<sub>3</sub> exposure

Meteorological datasets, with a consistent hourly-daily temporal resolution, were selected for two locations in Germany (Bremen) and Spain (Jerez), encompassing different climatic conditions. The sensitivity of two types of crops was assessed: wheat, which is relatively sensitive to O<sub>3</sub> damage, and barley, which is less sensitive. These two crops were exposed to a range of hypothetical O<sub>3</sub> mixing ratios of 20, 40, and 60 ppb during the entire crop growth cycle, as well as during specific months. Two agro-managements options were analysed: a potential yield case (i.e. no water stress by mimicking a full crop irrigation case), and a rain-fed case. Irrespective of ozone, rainfed wheat and barley yields are lower by only 12 % in Bremen compared to fully irrigated crops, while strongly reduced by 55 % in Jerez. Additionally, wheat yield losses, up to 30 % are calculated for ozone concentrations of 60 ppb, and only half of these for barley. Yield losses are substantially smaller in Jerez for rain-fed crops, when stomatal closure is limiting gas exchange, and thus impeding photosynthesis, crop growth and yields, but also reducing ozone uptake.

General findings are:

- Crop damages due to O<sub>3</sub> exposure increase with O<sub>3</sub> concentration
- Effects of high O<sub>3</sub> concentrations are very heterogeneous depending on month, site, crop and the simulated variable considered
- The highest impact is obtained when the month with high O<sub>3</sub> concentration coincides with the anthesis/*grain filling* stage (June for Bremen, April for Jerez)
- Rain-fed crop damage is more marked in Bremen than Jerez and irrigation practice exacerbates O<sub>3</sub> damages, especially in Jerez
- Barley is less affected by O<sub>3</sub> impact according to the lower sensitivity of the crop.

The algorithms developed can easily be implemented in other (generic or crop-specific) models of similar complexity.

Compare model results against field data under diverse conditions will be the next phase of this work, and further model developments are needed to simulate so-called “stomatal sluggishness” (i.e. damage to the stomata due to ozone).

## 1. Introduction

Tropospheric ozone is a photochemically produced secondary pollutant whose precursors are nitrogen oxides (NO<sub>x</sub>), methane and other volatile organic compounds and carbon monoxide. There is a wealth of evidence that at ground level, ozone is phytotoxic to plants, and can cause substantial damage to crops [Mills et al., 2007; Ainsworth et al, 2012]. Empirical evidence and model-based assessments suggest a large impact on crop yields globally, yet with marked variations across regions and with intricate interactions with climate change impact, adaptation and mitigation actions [Van Dingenen, et al., 2009; Burney and Ramanatan, 2014; Tai et al, 2014]. Ozone concentrations are already high in important cropland areas in North America, Europe, and South and East Asia. Concentrations are increasing rapidly in developing countries and are projected to continue to increase in coming decades. However, the effects of ozone pollution are currently not considered in most crop models, including the WOFOST model, currently implemented in the BioMA framework, and used in the JRC MARS crop forecasting activity. Consequently, ozone effects are excluded from model predictions of regional crop growth and yield. A particular gap in our understanding is how ozone interacts with other stresses that effect crop growth, such as soil fertility, CO<sub>2</sub> fertilization, soil water stress, heat stress and even pests and diseases (e.g. ozone has been shown to make crops more vulnerable to attack by pests such as red spider mite). Nevertheless, there is sufficient information on the effect of ozone on crop physiology, particularly how it influences photosynthesis, C allocation and early senescence to warrant the development of ozone modules that could be embedded within existing crop models.

Based on the results of an expert contract with (Confalonieri, 2016) during the first semester of 2016, this report describes the work of experts from the University of Milano in collaboration with JRC, to include ozone in the BioMA modelling framework, to integrate it with the WOFOST model and to provide detailed meteorological datasets for testing the models.

The report is structured as follows:

Section 2 describes which version of the WOFOST model was used for this study and for which reasons; and which interaction mechanisms between ozone and plant growth were included in the ozone module.

Section 3 describes the test conditions that were designed to evaluate the sensitivity of the extended model.

Section 4 describes the new ozone effect algorithms implement in the

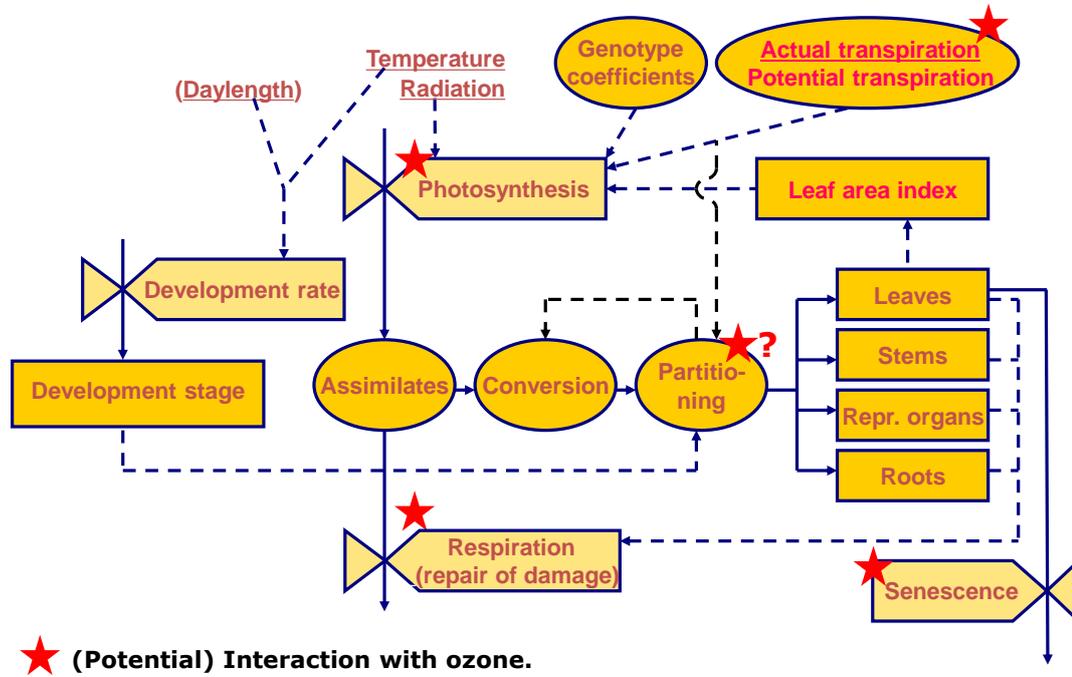
Section 5 describes the results of the preliminary modelling experiments that were conducted for the test conditions described in section 3.

Section 6 present recommendations and conclusions of the study.

## 2. Selection of WOFOST version and interaction mechanisms to study ozone effects on crops

Extensive experimental studies highlight the deleterious effects of chronic O<sub>3</sub> exposure on crop yields (Ainsworth et al., 2012). In such conditions, crop productivity is affected by a decreased CO<sub>2</sub> assimilation at leaf level (Amax; e.g. Feng et al., 2008) and a decreased synthesis of non-structural carbohydrates (i.e. sucrose, starch and pectins). These impacts on primary metabolism are partly responsible for the reduction of leaf area, a common response of field crops to O<sub>3</sub> enriched air (e.g., Morgan et al., 2004; Pang et al., 2009). In addition to lower carbon fixation, plants exposed to O<sub>3</sub> often display i) higher respiration rates (e.g., Amthor, 1988; Biswas et al., 2008), ii) altered biomass partitioning with decreased root biomass and redistribution of photosynthates from non-reproductive plant organs to grains and iii) a reduced leaf lifespan triggered by the acceleration of leaf senescence. All these responses contribute to the overall decrease in growth and yield. Interestingly, most of the processes affected are explicitly simulated by the WOFOST model (Diepen et al., 1989), which thus provides a suitable framework to integrate available models accounting for O<sub>3</sub> limitations within a crop growth model. Currently, two versions of WOFOST are implemented in BioMA (Stella et al., 2014; de Wit, 2014). They differ in the way by which they define the dependence of crop parameter values on air temperature and phenological development. The original WOFOST adopts so-called AFGEN tables to allow users to define arbitrary functions, which linearly interpolate between values of a dependent variable, Y, given a value of an independent variable, X, and a table of X and Y data pairs. In the new WOFOST-GT, such relations are described by simple mathematical equations, thus reducing model complexity and the number of parameters. Even though the second approach is deemed more elegant and sounder (since it reduces parameterization effort and the risk to fit unrealistic functions), we opted for using the original WOFOST which provides more flexibility and for which parameter sets are available which are widely used, including in the JRC MARS crop forecasting system. WOFOST is a generic crop simulator for annual field crops, based on a hierarchical distinction between potential and water-limited production. It performs its calculations with a one-day time step, using Euler integration to calculate the values of its state variables at the end of each day. Crop development rate is simulated as a simple function of temperature, photoperiod or both thermal and photoperiodic conditions. Photosynthesis (gross CO<sub>2</sub> assimilation) is simulated on the basis of intercepted photosynthetically active radiation (PAR). Fluxes of direct and diffuse PAR are computed using Lambert-Beers law to estimate the light distribution in the canopy. The extinction coefficient for solar radiation can be customized according to the canopy architecture of the simulated crop. Maintenance respiration is assumed to be proportional to the dry weight of the plants organs, considering that different organs have different respiration/weight ratios depending on their composition. Assimilated carbon is partitioned among the different crop organs according to partitioning coefficients, modulated according phenological development. In this process, losses associated with conversion and growth respiration are accounted for. The daily increase in total LAI is estimated using a two-stage approach: using an exponential function driven by temperature during early growth phases, and from specific leaf area (SLA) and daily increase in leaf dry weight later on. LAI is then distributed within the canopy according to Gaussian Integration distances. Non-photosynthesis (dead) LAI units are computed daily

as a function of self-shading and senescence. A diagram showing the main processes accounted for by the WOFOST model and the possible coupling points to an idealised model reproducing the effects of O<sub>3</sub> on plant growth is shown in Figure 1.



**Figure 1. Flow chart of the processes implemented in the WOFOST model. Red stars indicate the processes that are subjected to ozone effects**

Some adaptation to the model is required to enable consistent estimates of O<sub>3</sub> damages. In the BioMA framework, this is done within the so-called AbioticDamage component. An overview of adaptations considered is given in Table 1.

First, it is important to note that O<sub>3</sub> damage largely depends on the flux of the gas into plant tissues, which, in turn, is largely controlled by stomatal aperture. This means that either WOFOST or the O<sub>3</sub> impact models that will be plugged into the modelling solution have to calculate stomatal conductance (transpiration is using Penman- CO<sub>2</sub> fluxes =H<sub>2</sub>O flux). Although different models are available in literature (e.g. Leuning 1995; Medrano et al., 2002; Tuzet et al., 2003), the approach used by AquaCrop (Raes et al., 2009) seems to represent the best trade-off among the i) compatibility with the level of detail used by WOFOST to represent crop processes, ii) availability of input data usually stored in agrometeorological databases, iii) the availability of sets of proved parameters to differentiate crop-specific responses to water stress.

Moreover, even though WOFOST currently updates state variables with a daily time step, it could be important to estimate the O<sub>3</sub> movement into the mesophyll (controlled by stomata) at a shorter integration time step. The calculation of hourly fluxes could be a viable solution. The main reason for this is related to the diurnal variation of both O<sub>3</sub> tropospheric concentration – rising with high sunlight and temperature – and stomatal conductance, which are often coupled and sometimes decoupled (e.g., when excess light and temperature cause at the same time depression of photosynthesis and high O<sub>3</sub> concentrations). This could be managed by calculating, for all the groups of emitted GAI (green leaf area index) units

having the same age, O<sub>3</sub> fluxes at hourly time step in the range of the daylight hours and then averaging the sum of hourly fluxes on the total number of contemporaneous age classes in the day. Daily averaged fluxes were then used to compute the O<sub>3</sub>-induced fractional reduction of daily photosynthesis rates as simulated by WOFOST model. Another solution could be to convert WOFOST to hourly time step for all assimilation processes; which however was not yet possible with the time and resources allocated for this project. A case study comparing methods should be considered.

While O<sub>3</sub> uptake depends on stomatal conductance, it is also known that O<sub>3</sub> can affect stomatal conductance. This can be a reducing effect (Morgan et al., 2003), probably because of the reduced photosynthesis and the related increase of CO<sub>2</sub> concentration in the mesophyll, or because of the formation of plant hormones in response to ozone, such as ethylene, which induces stomatal closure. Another key aspect in modulating stomatal conductance and O<sub>3</sub> damages is water uptake: different experiments corroborate the hypothesis that drought mitigates the impact of O<sub>3</sub> by causing stomatal closure, thus reducing O<sub>3</sub> flux into leaves. On the other hand, Wilkinson and Davies (2009) highlight an increasing effect, attributed to the loss of functionality of stomata in O<sub>3</sub>-stressed plants, which remain open despite drought stress. This phenomenon, often referred to as ozone-induced stomatal sluggishness, has the potential to sensibly change the carbon and water balance of crops (Paoletti and Grulke 2005). Several approaches were inspected to understand their potential impact, were they to be implemented in the ozone model. The approach of Hoshika et al. (2015) (see table 1) appears to be promising but would require validation for its applicability to annual crops prior to its implementation.

Ozone is usually detoxified in plants at uptake rates below a critical threshold, above which the rate of photosynthesis decreases. The ability of crops to resist to low ozone concentrations via detoxification and repair is strictly dependent on leaf age (Alsher and Amthor 1988), with young leaves being able to tolerate higher O<sub>3</sub> concentrations and completely repair from damage in a relatively short time (from hours to days) depending on the cultivar and pedoclimatic conditions (Pell et al., 1997). Nevertheless, prolonged exposure to even low O<sub>3</sub> concentrations is responsible for enhancing rates of leaf senescence, thus reducing the period during which plants can recover from ozone damage.

In any case, reliable estimates of drought stress and its impact on stomatal conductance requires the simple single-layer soil-water-plant-uptake approach of the WOFOST model to be replaced by a more elaborated soil water redistribution and uptake model; for example those implemented within the software component UNIMLSoilW. For this study we decided to adopt:

- A multi-layer cascading approach (Ritchie, 1998) to simulate the downward movement of water through the soil profile: water fills up the layers until field capacity is reached, with the fraction exceeding this threshold moving to the deeper layer.
- The EPIC (Williams et al., 1989) approach to calculate root water uptake from each layer, requiring rooting depth, soil water content and crop potential transpiration as input variables.

These approaches appear suitable for the purpose of this study, since their limited input requirements are consistent with data availability over large scales.

**Table 1. Inspected biophysical processes, model approaches and modifications needed to couple the original approaches to the BioMA AbioticDamage O<sub>3</sub> model. I: implemented; NI: not implemented.**

Biophysical process	Model approaches and modifications	Action
1.2.1.1.1.1.1 Effect of water stress on stomatal conductance	1.2.1.1.1.1.2 A water stress related factor that multiplies the stomatal conductance (0 =maximum reduction; 1 = no effect) is introduced in the algorithm computing O <sub>3</sub> fluxes already implemented in the original O <sub>3</sub> model available in the AbioticDamage component. following the approach used by AquaCrop (Raes et al., 2009).	1.2.1.1.1.1.3
Reduction of carboxylation rate of rubisco	According to Ewert and Porter (2000). Decreases in rubisco-limited rate, distinguish between i) immediate effects due to high ozone fluxes and ii) long terms effects driven by leaf senescence acceleration. Since decreases in daily rate of gross photosynthesis are implicitly induced by the reduction in GAIs associated to the faster ageing of each contemporaneous class of GAI units, the average long-term reducing factor will not be applied to further reduce the actual daily gross CH <sub>2</sub> O assimilation rate calculated by WOFOST. The rationale for this is to reduce the risk of markedly overestimating the effect of senescence on reducing photosynthesis rates, double counting its impact on plant growth.	1.2.1.1.1.1.4
1.2.1.1.1.1.5 Ability of plants to recover from ozone damage	According to Ewert and Porter (2000), the recovery from ozone-induced damage in a given day is used to modulate the ozone impact on rubisco-limited rate of photosynthesis at light saturated conditions of the following day, depending on leaf age. Since WOFOST considers LAI emitted units, instead of individual leaves, recovery factors are computed each day for all LAI units with the same age.	I
Metabolic cost (Increased respiration) to avoid or repair ozone damage		NI

<p>1.2.1.1.1.1.6 Acceleration of leaf senescence due to O<sub>3</sub> exposure</p>	<p>1.2.1.1.1.1.7 Enhanced rates of senescence induced by prolonged exposure to O<sub>3</sub> in a given day is computed daily for each GAI unit of the same age class using reducing factors (0 = maximum reduction; 1 = no effect; unit less) calculated as function of cumulative ozone uptake (Ewert and Porter, 2000). An average indicator targeting the shortening of leaves lifespan due to ozone exposure is computed by averaging the sum of all daily factors on the total number of contemporaneous GAI age classes.</p>	<p>1.2.1.1.1.1.8</p>
<p>1.2.1.1.1.1.9 Reduction of green leaf area index due to foliar chlorosis or necrosis induced by O<sub>3</sub></p>	<p>1.2.1.1.1.1.10 An extensive literature search needs to be carried out to find out approaches that are i) coherent (neither too rough nor too refined) with the level of detail used by WOFOST and O<sub>3</sub> models and ii) use standard input variables. As an alternative, if measured data are available from literature, one could derive generic response functions triggered by a crop-specific sensitivity parameter set to 0 (or to 1) in case of no impact.</p>	<p>1.2.1.1.1.1.11</p>
<p>1.2.1.1.1.1.12 Stomatal sluggishness</p>	<p>1.2.1.1.1.1.13 The approach from Hoshika et al. (2015) accounts for the effect of chronic exposure to ozone on stomatal sluggishness by progressively increasing the minimum crop-specific stomatal conductance via a sigmoid function having the cumulative ozone uptake as independent variable. This model, as is, cannot be coupled directly with the AbioticDamage ozone model; but its implementation could be considered to modulate for instance the instantaneous O<sub>3</sub> leaf uptake over a plant-specific threshold (UO<sub>&gt;FO3crit</sub>) according to the following equation:</p> $UO_{\text{Slug}} = UO_{>FO3\text{crit}} \cdot \frac{g_{\text{min}S}}{g_{\text{min}}}$ $UO_{\text{Slug}} = UO_{>FO3\text{crit}} \cdot \frac{g_{\text{min}S}}{g_{\text{min}}}$ <p>1.2.1.1.1.1.14 Where: <math>g_{\text{min}}</math> (mol m<sup>-2</sup> s<sup>-1</sup>) is the minimum stomatal conductance in the</p>	<p>1.2.1.1.1.1.16</p>

	<p>absence of O<sub>3</sub>; <math>g_{\min S}</math> (mol m<sup>-2</sup> s<sup>-1</sup>) is the minimum stomatal conductance accounting for stomatal sluggishness as computed by Hoshika et al. (2015).</p> <p>1.2.1.1.1.15 A strong limitation of Hoshika's approach is an empirical relationship developed for temperate deciduous forests and thus needs to be validated against measured data on herbaceous crops before being used outside the conditions for which it was calibrated.</p>	
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### 3. Test conditions to evaluate the sensitivity of the modelling solution to ozone exposure

A set of synthetic test conditions was generated to assess the crop model response in a range of environmental conditions for different crops, to verify model behaviour and to allow intercomparison with other models.

A first set of simulations was set up for two winter cereals with distinct tolerance to O<sub>3</sub> and environmental characteristics (such as different O<sub>3</sub> atmospheric concentrations). The two crops considered markedly differ in the sensitivity to ozone damage - i.e. winter wheat (susceptible) and winter barley (tolerant) – but share many phenological and productive traits<sup>1</sup>. This approach will greatly facilitate the analysis of results, allowing to separate the effects of O<sub>3</sub> exposure on crops from any possible interference due to interspecific differences in crop development and growth. Simulations were performed for two locations: 1) Bremen, in northwestern Germany, with a marine temperate humid climate and high yield potential, and 2) Jerez de la Frontera, Spain with Mediterranean climate with average-low yield potential. For each region, 20-years time series of meteorological data were selected [Table 4] to run simulations under rain-fed as well as under fully irrigated conditions. In this way, the potential interaction of ozone with drought conditions is explored (e.g., Morgan et al., 2003; Feng et al., 2008). Furthermore, such sample size is deemed large enough to capture the short-term random fluctuations – such as daily weather variations –, seasonal and interannual variability, as well as most part of the less frequent climate events that may occur in a given agro-ecosystem (Semenov and Barrow 2002). In this context simulations are performed by considering a sandy-loam soil, with a relatively low water holding capacity. Two reference levels of ozone concentrations are chosen: a sustained (without any daily or monthly variation) background ozone of 40 ppb and an elevated ozone of 60 ppb, respectively representative for background (inflow) O<sub>3</sub> and elevated continental O<sub>3</sub> concentrations (Feng and Kobayashi, 2009). As current model calibrations may implicitly include some effect of ozone in the parameterization, simulations were also performed using a pre-industrial ozone concentration – i.e. 20 ppb – as reference control, to test the model in presence of negligible ozone damages. For this first analysis synoptic and diurnal variations of ozone are ignored, as they may complicate the analysis. We note that this range also encompasses future (2030) annual ozone levels under a variety of scenarios for 2000-2030-with projected regional changes ranging from ca. -8 to +15 ppb - depending on scenario and region considered (Figure 2; Fiore et al., 2012; Kirtman et al., 2013).

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<sup>1</sup> The same parameterization is operatively used for both crops within the JRC MARS crop growth monitoring system (CGMS)

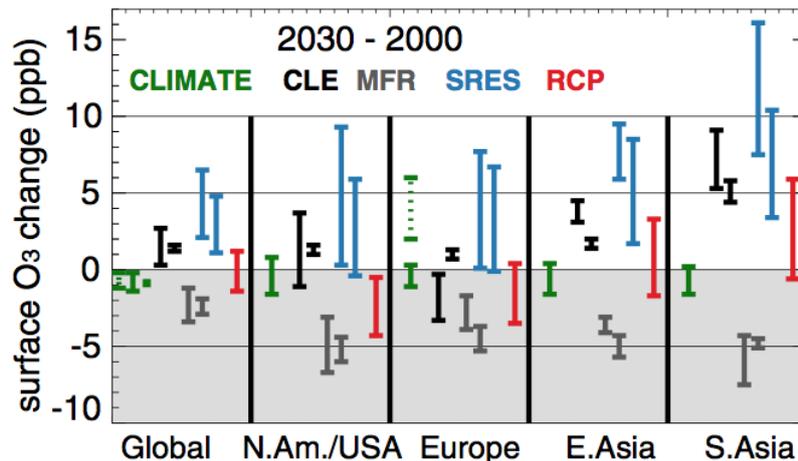


Figure 2. Changes in surface O<sub>3</sub> (ppb) between year 2000 and 2030 driven by climate alone (CLIMATE, green) or driven by emissions alone, following current legislation (CLE, black), maximum feasible reductions (MFR, grey), SRES (blue) and RCP (red) emission scenarios. Results are reported globally. Where two vertical bars are shown (CLE, MFR, SRES), they represent the multimodel standard deviation of the annual mean based on the Atmospheric Composition Change: a European Network (ACCENT)/Photocomp study (Dentener et al., 2006) and (right bar) the parametric HTAP ensemble (Wild et al., 2012; four SRES and RCP scenarios included). Under Global, the leftmost (dashed green) vertical bar denotes the spatial range in climate-only changes from one model (Stevenson et al., 2005) while the green square shows global annual mean climate-only changes in another model (Unger et al., 2006). Under Europe, the dashed green bar denotes the range of climate-only changes in summer daily maximum O<sub>3</sub> in one model (Forkel and Knoche 2006). Source Kirtman et al., 2013 in IPCC-AR5 report.

In addition to examining the effects on crop growth and yield of constant ozone concentration throughout the growing season, we also tested the model response to monthly variations in O<sub>3</sub> concentration. For this purpose all months are set at the background ozone level (i.e. 40 ppb), except one, which is set at high ozone concentration (i.e. 60 ppb). Simulations are performed iteratively by changing each time the month displaying high O<sub>3</sub> concentrations, in order to identify the most critical phases of the crop cycle with regards to ozone exposure. The synopsis of the conditions explored is provided in Table 2; the total number of simulations (56) is determined by all the possible combinations of the factors and levels tested.

**Table 2. Factors and levels tested in the first phase of the simulation experiment. Total number of simulation is 64.**

<b>Factor</b>	<b>Levels</b>
Crop	Winter C3 (wheat, barley)
O <sub>3</sub> susceptibility	Tolerant (winter barley)
	Susceptible (winter wheat)
Climate	Marine
	Mediterranean
Precipitation	Rainfed
	Full irrigated
Soil texture	Medium/sandy-loam
	20 whole cycle
O <sub>3</sub> concentration (ppb)	40 whole cycle
	60 whole cycle
	60 February
	60 March
	60 April
	60 May
	60 June

For each combination of conditions tested, selected model output is stored (Table 4) to gain insight into the modelled effect of ozone damage on crop growth and productivity. In particular, daily values of aboveground biomass, green leaf area index and storage organs biomass are used as key variables influenced by photosynthesis activity. Variables related to water use, such as daily and cumulative evapotranspiration and water stress index (i.e., the ratio between potential and actual transpiration), are used to distinguish the impacts of losses due to water stress and stomatal closure from the losses due to ozone exposure. Final yield, harvest index and total water use are chosen as the synthetic variables describing crop productivity. Furthermore daily and cumulative O<sub>3</sub> fluxes to stomata and the percentage reduction of daily assimilation rates are tracked to separately inspect the effects of short- and long-term exposure to O<sub>3</sub>. A summary of data needed as input for the modelling solution and simulated outputs is given in Tables 3 and 4.

**Table 3. List of inputs needed to run the modelling solution under the test conditions defined in Table 1. Inputs are grouped in three classes, related to i) daily meteorological data, ii) crop management data and iii) Soil properties initialization data.**

<b>Inputs</b>	<b>Unit</b>
<i>Daily meteorological data</i>	
Maximum air temperature	°C
Minimum air temperature	°C
Cumulative precipitation	mm
Average wind speed	mm s <sup>-1</sup>
Minimum relative air humidity	%
Maximum relative air humidity	%
Global solar radiation	MJ m <sup>-2</sup> d <sup>-1</sup>
Reference evapotranspiration	mm
Latitude	°
Tropospheric Ozone concentration	ppb
<i>Crop management data</i>	
Sowing date	doy
Irrigation starting date	doy
Harvest date	doy
<i>Soil properties initialization data</i>	
Horizon thickness	m
Volumetric water content at saturation	m <sup>3</sup> m <sup>-3</sup>
Volumetric wilting point	m <sup>3</sup> m <sup>-3</sup>
Volumetric field capacity	m <sup>3</sup> m <sup>-3</sup>
Saturated hydraulic conductivity	mm h <sup>-1</sup>
Bulk density	t m <sup>-3</sup>
Texture*	%
Number of layers	-
Layer thickness	m
Skeleton	%

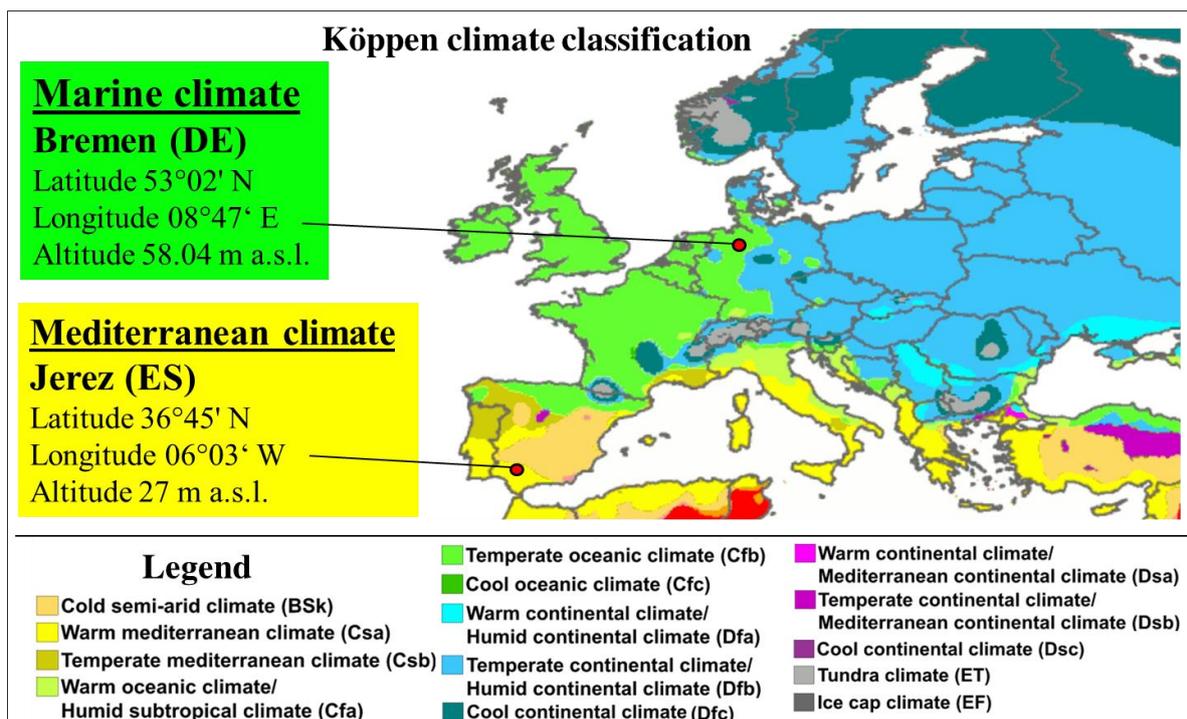
\* percentage of clay, silt and sand

**Table 4. List of simulated outputs analyzed. Variables are grouped in three classes, related to i) water management, ii) crop productivity and iii) ozone damage to crop.**

<b>Simulated output</b>	<b>Unit</b>
<i>Water management</i>	
Daily $ET_0$	$mm\ d^{-1}$
Cumulative $ET_0$	mm
Water stress index	-
Water stress effect on stomatal conductivity	-
<i>Crop productivity</i>	
Daily aboveground biomass	$kg\ ha^{-1}$
Daily green leaf area index	$m^{-2}\ m^{-2}$
Final yield	$kg\ ha^{-1}$
Harvest index	-
Cumulative water uptake	mm
<i>Ozone damage</i>	
Instantaneous $O_3$ fluxes to stomata	$nmol\ m^{-2}\ s^{-1}$
Cumulative $O_3$ fluxes to stomata	$nmol\ m^{-2}$
Percentage $A_{max}$ reduction	%

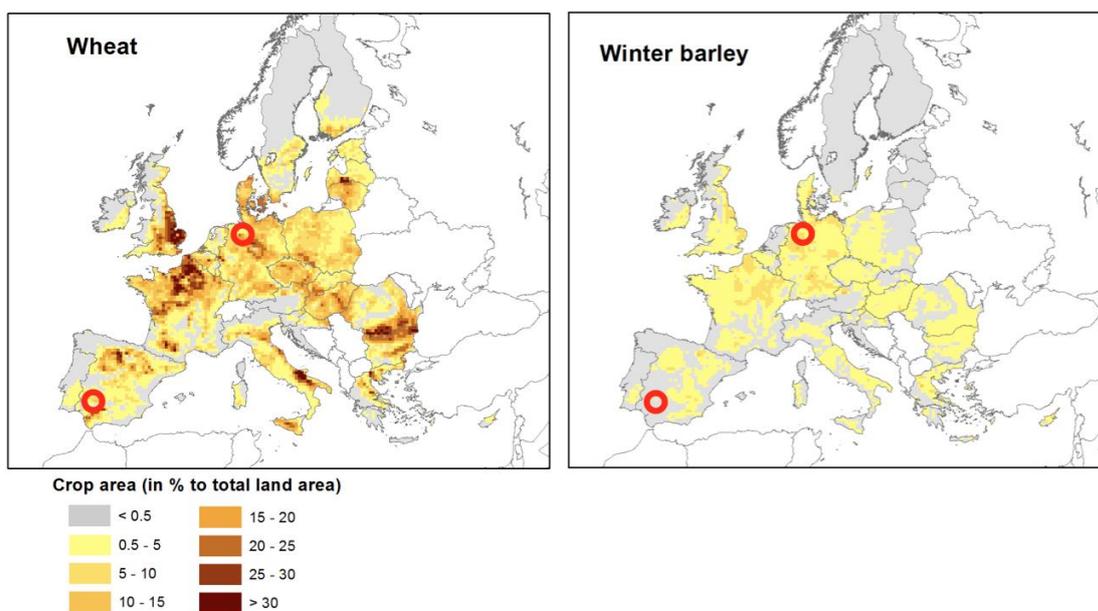
$ET_0$ : reference evapotranspiration;  $A_{max}$ : maximum leaf  $CO_2$  assimilation rate ( $Kg\ ha^{-1}\ h^{-1}$ ), WOFOST parameter.

In order to identify eligible test sites where to perform the first phase of simulation experiment, we crossed the information from the i) European climate classification according to the Köppen-Giger taxonomy (Figure 3; Peel et al., 2007), ii) maps of wheat and barley production area coverage and productivity by country (Figure 4; Bioma, 2016; FAOSTAT 2016), iii) the within country percentage cover occupied by selected species (USDA 2016), iv) the presence of reliable, consistent and accessible data sources, able to provide long time series of meteorological data, essential as input for the modelling solution.



**Figure 3. Map of European climate and sites selected as representative for Marine and Mediterranean climates.**

As result, data from meteorological stations located close to Bremen, in northwestern Germany, and to Jerez de la Frontera, in south-western Spain, were selected as representative for Marine and warm Mediterranean climate. By analyzing data on the average production quantities by country available in the FAOSTAT database in the period 1993-2013, both countries prove to be among the top wheat and barley producers in the EU-27 (Figure 4).



**Figure 4. Crop area- production area for wheat and barley (<http://bioma.jrc.ec.europa.eu>). Red circles represent the sites selected to run the first set of simulations.**

The economic importance of the two winter cereals in the target sites is confirmed by the high percentage of wheat and to a smaller extent barley harvested area in the region/state of belonging (Figure 4).

It can be noticed that the selected crops markedly differ in the average yields achieved, according to the crop suitability to pedo-climatic conditions in the target areas. While yields in Niedersachsen, around Bremen, fluctuate around  $7.5 \text{ t ha}^{-1}$  ( $\pm 0.52 \text{ t ha}^{-1}$ ) for wheat and  $6.0 \text{ ha}^{-1}$  ( $\pm 0.54 \text{ t ha}^{-1}$ ) for barley, in Andalucia (Jerez de la Frontera) both crops show average yields of about  $2.9 \text{ t ha}^{-1}$  with a standard deviation ranging from  $0.49 \text{ t ha}^{-1}$  to  $0.57 \text{ t ha}^{-1}$ .

For both sites, daily maximum and minimum air temperature ( $^{\circ}\text{C}$ ), precipitation (mm), average wind speed ( $\text{m s}^{-1}$ ) and relative air humidity (%) were extracted from the European Climate Assessment & Dataset (ECA&D; <http://eca.knmi.nl/>). Global solar radiation ( $\text{MJ m}^{-2} \text{ d}^{-1}$ ) and reference evapotranspiration ( $\text{ET}_0$ ; mm) were generated according to Hargreaves (Hargreaves and Samani 1982) and FAO (Allen et al., 1998) equations respectively. The monthly patterns of meteorological variables collected within the period 1996-2015 were then analyzed; some synthetic previews are shown in Appendix (Figure 1 and 2). In addition, the above listed daily data were used to generate hourly values of meteorological drivers, in order to produce an hourly meteorological dataset consistent with the daily one, to be used as input to the hourly time step  $\text{O}_3$  models for future intercomparisons. To generate synthetic hourly data, the following approaches were adopted:

- hourly air temperature: Campbell (1985);
- hourly air relative humidity: Waichler and Wigmosta, 2003;
- hourly wind speed: Mitchell et al., 2000;
- hourly rainfall: Meteotest 2003;
- hourly radiation: Chen et al., 1999;
- hourly reference evapotranspiration: Allen et al., 1998.

An overview of weather variables patterns in both sites is given in Appendix A.

### **Options for future work:**

Once results will be definitive, the reference simulation protocol could be reiterated on the same crops by changing soil texture and/or adopting more realistic patterns of monthly mean surface ozone concentrations (e.g., Avnery et al., 2011). As an alternative, the setup of simulation experiment could be applied to other C3 species or even to C4 summer crops (extending to September), which generally show a lower sensitivity of plant growth to  $\text{O}_3$  concentrations than C3 species (Table 3; Sitch et al., 2005).

## 4. The modelling solution and modifications to the AbioticDamage component

### 4.1. The modelling solution

The third phase of the workflow dealt with the realization of a customized modelling solution for the simulation, with daily time step, of ozone ( $O_3$ ) damages to crops. The developed modelling solution links (i) the original WOFOST version implemented in the software component UNIMI.CropML, (ii) soil water redistribution and uptake models collected by UNIMI.SoilW and (iii) the amended ozone impact model present in UNIMI.AbioticDamage (Figure 5).

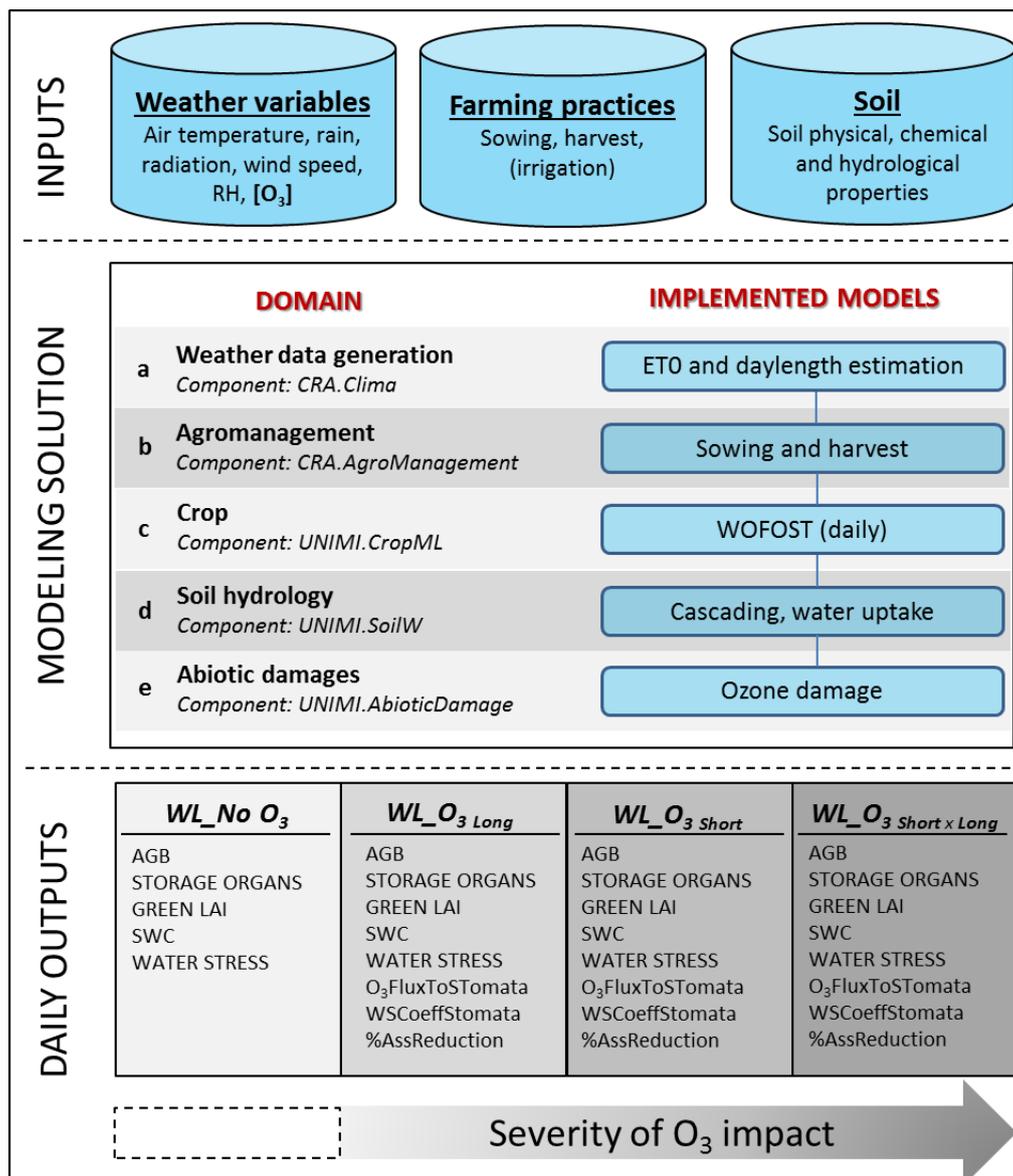


Figure 5. Schematic representation of the models composing the modelling solution and the components they belong to.

The CropML\_SoilW\_AbioticDamage\_solution project handles the interactions between the I/O data produced by models belonging to the software components, in order to simulate the

different biophysical processes shown in Figure 5. The entry point of the modelling solution is the RunnerAPI class, containing instances of Adapter classes (Gamma et al., 1994) and managing their call. Adapter classes, in turns, encapsulate the logic to perform dynamic simulations, by calling specific models selected among those provided by software components. The components implemented in the modelling solution communicate in each integration time step (daily), via the methods provided by ISimulationComponent interface. Information produced during the simulation is stored in dedicated classes i.e., DataTypes, containing the instances of the data structures of the components implemented in the modelling solution. DataTypes are also used to store input data from different sources (e.g., meteorological data, pedological information). All DataTypes are shared by all the Adapter classes of the MS, making possible the communication of models belonging to different domains, meant as the possibility of exchanging variables among software components. The Adapter class of the component CRA.AgroManagement is able to publish specific events (e.g., planting, harvest), which are listened by other Adapters via the HandleEvents method of the ISimulationComponent interface.

## 4.2. Input data layers

The data needed as inputs to the CropML\_SoilW\_AbioticDamage\_solution are organized in information layers and integrate data from different sources, allowing an ease coupling with biophysical models.

- **Weather** layer contains .txt files collecting daily meteorological data covering the whole simulation period for the site to be tested. Weather variables included in the sample weather file used to test the modelling solution are the following: daily minimum and maximum air temperatures ( $^{\circ}\text{C}$ ), rainfall (mm), average wind speed ( $\text{m s}^{-1}$ ) global solar radiation ( $\text{MJ m}^{-2} \text{d}^{-1}$ ) minimum and maximum relative humidity (%) and Ozone concentration (parts per billion, ppb).
- **Farming practices** layer is represented by a single .xml file which currently includes the crop species grown, the sowing and harvest date and the planting depth for each combination site  $\times$  year. This layer can be modified and/or extended by the user by specifying different sets of rules and impacts to simulate alternate management strategies.
- **Soil** layer is made up by an .xml file collecting the parameters to set the physical and hydrological properties along the soil profile at the beginning of simulation. Main soil properties concern: horizon thickness (m), volumetric water content at saturation ( $\text{m}^3 \text{m}^{-3}$ ), volumetric wilting point ( $\text{m}^3 \text{m}^{-3}$ ), volumetric field capacity ( $\text{m}^3 \text{m}^{-3}$ ), saturated hydraulic conductivity ( $\text{mm h}^{-1}$ ), bulk density ( $\text{t m}^{-3}$ ), texture (i.e. relative percentage of clay, silt and sand; %), skeleton (%), number of layers (unit less) and layer thickness (m).

## 4.3. The modelling layers within the modelling solution

Approaches implemented in each modelling layer are outlined in the following list:

- a. **CRA.Clima** is used to estimate reference evapotranspiration according to the Hargreaves equation (Hargreaves and Samani, 1985), which requires daily minimum and maximum temperature and extra-terrestrial solar radiation as input. The latter is calculated by the component as an integration of hourly radiation estimated from the solar constant, zenith

angle and a correction parameter specific for each day of the year. Day length is estimated as function of latitude and solar declination.

- b. **CRA.AgroManagement** triggers the occurrence of agricultural operations at run time according to (i) set of rules based on management decisions (e.g., scheduled events) and/or some states of the system. This components currently handles – within the solution – sowing and harvest operations, with the possibility of including dedicated rules to manage irrigation events according to the method (e.g. sprinkler, surface flow, drip or flood irrigation) and the scheduling time needed (i.e. turn or plant needs based irrigation). For instance, the fully irrigated treatment as defined in the test condition report (no stress due to water shortage), was reproduced here according to an automatic rule which triggers an irrigation event every time that the water stress index is lower than one, bringing the volumetric soil water content in the rooted soil back to field capacity.
- c. **UNIMI.CropML** implements the model WOFOST. Crop development is simulated as a thermal-driven process. Instantaneous gross CO<sub>2</sub> assimilation is estimated in three moments during the day as a function of intercepted radiation and of a photosynthesis-light response curve of individual leaves. Light interception depends on total incoming radiation, on photosynthetic leaf area and on leaf angle distribution. Canopy architecture is divided into three horizontal layers with LAI split among them using Gaussian integration. Biomass partitioning is driven by partitioning factors and efficiencies of assimilates conversion into the different organs (i.e., growth respiration). Daily increase in total LAI is estimated as a function of temperature during early growth whereas it is derived from specific leaf area and development stage later on. Non-photosynthetically active (dead) LAI units are computed each day as a function of canopy self-shading and senescence. Potential evapotranspiration is estimated using the Penman approach (Frere and Popov, 1979), and water stress is derived by the actual to potential transpiration ratio.
- d. **UNIMI.SoilW** is used to simulate soil water redistribution among soil layers according to a cascading (tipping bucket) approach. The changes of soil water content and fluxes among layers are provided as output; water percolating from the bottom layer is lost from the soil column. The component also estimates root water uptake based on evapotranspiration demand, soil water content and variable root depth. The component does not simulate water infiltration. Input water is assumed to be net rain able to infiltrate the soil. No attempt to compute runoff, plant and mulch interception is performed. The component also allows the simulation of effective plant transpiration, soil evaporation and the effects of soil tillage and subsequent settling of hydrological properties of the soil (field capacity, wilting point, retention functions, conductivity functions, bulk density). The latter are not taken into account in the current modelling solution.
- e. **UNIMI.AbioticDamage** contains a complex model for the simulation of the crop damages due to ozone. It implements a model of leaf aerodynamic and boundary layer resistance (Spiker et al., 2007), the calculation of average leaf conductance proposed by Georgiadis et al. (2005), and the fractional reduction of plant production in function of the ozone flux through the stomata and the leaf conductance of water, according to the approach proposed by Sitch et al. (2005).

#### 4.4. UNIMI.AbioticDamage modifications

As discussed in section 2 of this report (Selection of WOFOST version and interaction mechanisms to study ozone effects on crops), the O<sub>3</sub> model implemented in the UNIMI.AbioticDamage component has been modified to account for some O<sub>3</sub> effects on crop growth not considered in the original version.

#### 4.4.1. Effect of water stress on stomatal conductance

A water stress related factor modulating the stomatal conductance ( $K_s$ , 0 =maximum reduction due to water stress-induced stomatal closure; 1 = no effect; unitless) was introduced in the algorithm computing the instantaneous  $O_3$  leaf uptake over a critical threshold ( $UO_{>FO3crit}$ ; Equation 1, Sitch et al., 2005) to adjust  $O_3$  fluxes to stomata ( $FO_3$ ,  $nmol\ m^{-2}\ s^{-1}$ ).

$$UO_{>FO3crit} = \max[(FO_3 \cdot K_s - FO_{3crit}), 0] \quad UO_{>FO3crit} = \max[(FO_3 \cdot K_s - FO_{3crit}), 0] \quad [1]$$

Where:  $FO_{3crit}$ , ( $nmol\ m^{-2}\ s^{-1}$ ) is a plant-specific critical threshold below which the damage to tissues due to  $O_3$  leaf uptake is equal to 0. In other words, the lower the threshold, the higher is the plant susceptibility to  $O_3$  damage.

$K_s$  response function is computed according to the approach used in the model AquaCrop (Equation 2; Figure 5; Raes et al., 2009).

$$K_s = \begin{cases} 1 & \text{if } D_{rel} = 0 \\ 1 - \frac{e^{D_{rel} \cdot f_{shape}} - 1}{e^{f_{shape}} - 1} & \text{if } 0 < D_{rel} < 1 \\ 0 & \text{if } D_{rel} = 1 \end{cases} \quad [2]$$

Where:  $D_{rel}$  (%) is the fraction of water depleted in the root zone relative to the full amount the soil can hold between an upper ( $p_{upper}$ ) and lower ( $p_{lower}$ ) critical threshold of total available soil water (TAW);  $f_{shape}$  (unit less) is a crop specific parameter modulating the shape of the response curve (e.g. 2.5 for wheat, 6 for maize and sorghum, 3, for rice, potato and soybean, 2 for sunflower).

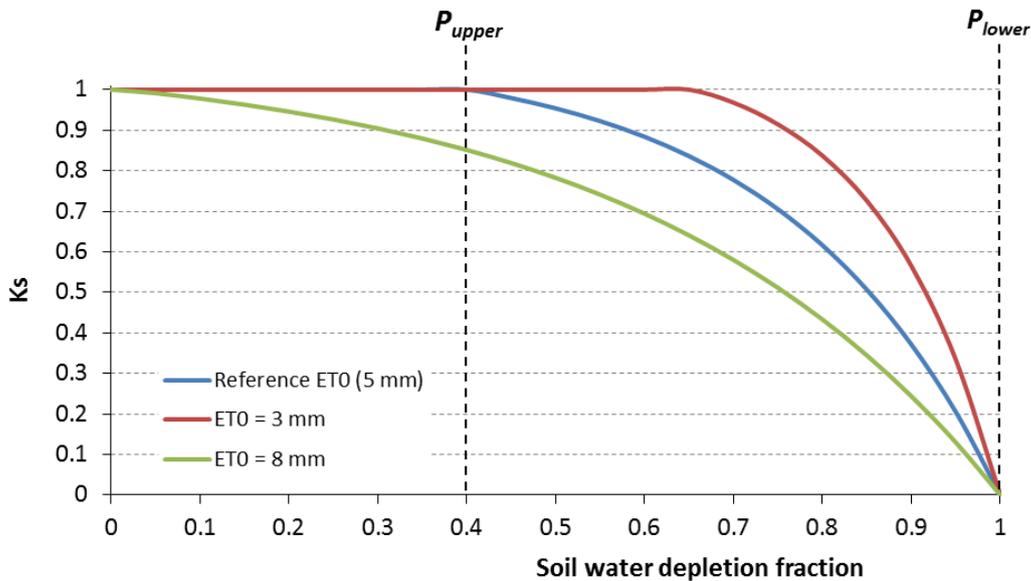


Figure 5. Stomatal conductance response function( $ks$ , unitless) to relative depletion of soil water and evapotranspiration demand.

The critical thresholds are expressed as a fraction of TAW, with the lower one set to permanent wilting point ( $p_{lower}=1$ );  $D_{rel}$  is computed according to equation 3.

$$D_{rel} = \frac{\left(\frac{FC - WC}{FC - WP}\right) - p_{upper}}{1 - p_{upper}} \quad D_{rel} = \frac{\left(\frac{FC - WC}{FC - WP}\right) - p_{upper}}{1 - p_{upper}} \quad [3]$$

Where: FC ( $m^3 m^{-3}$ ) is the volumetric soil water content at field capacity; WC ( $m^3 m^{-3}$ ) is the actual volumetric soil water content in the rooted zone; WP ( $m^3 m^{-3}$ ) is the volumetric soil water content at wilting point.

Tabular values for the upper threshold ( $p$ ) are given for different crops at a reference evaporative demand of  $ET_0 = 5 \text{ mm d}^{-1}$ ; for different levels of  $ET_0$ ,  $p_{upper}$  is adjusted at runtime according to the equation 4 (Raes et al., 2009).

$$0 \leq P_{upperadj} = p_{upper} + f_{adj} [0.04 \cdot (5 - ET_0)] \cdot \log_{10}(10 - 9 \cdot p_{upper}) \leq 1 \quad [4]$$

Where:  $f_{adj}$  (unit less, default value = 1) is a model parameter set to increase ( $>1$ ) or decrease ( $<1$ ) the  $p_{upper}$  adjustment.

The log term in the equation 4 amplifies the adjustment when the soil is wet compared to when it is dry, based on the likely restriction of stomata and transpiration (and thus a lower effect of the evaporative demand) when the soil is dry.

#### 4.4.2. Reduction of daily rate of gross photosynthesis

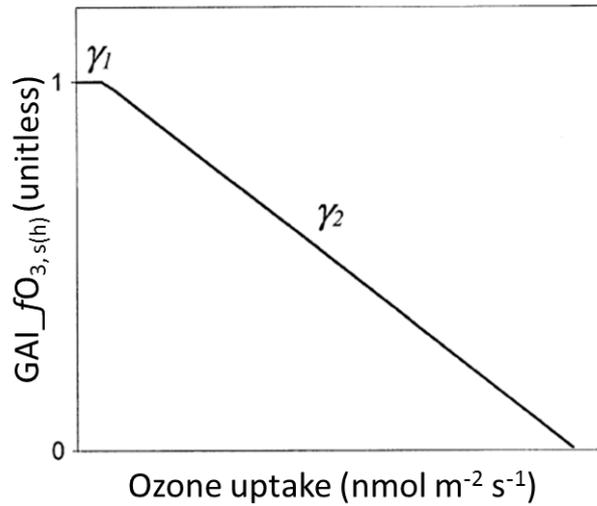
The library of  $O_3$  impact models on photosynthesis rates implemented in UNIMI.AbioticDamage component (Sitch et al., 2005) was extended by including the approach developed by Ewert and Porter (2000), which models the decreases in the hourly rates of net photosynthesis distinguishing between (i) immediate effects due to high ozone fluxes and (ii) long term effects driven by leaf senescence acceleration. In order to allow the new ozone impact model based on thea SUCROS approach of photosynthesis (Van Ittersum et al., 2003), originally developed for Farquhar (Farquhar et al., 1980), we applied the ozone damage factors to reduce the actual daily gross  $CH_2O$  assimilation rate, as driven by the maximum leaf  $CO_2$  assimilation rate ( $A_{max}$ ,  $Kg \text{ ha}^{-1} \text{ h}^{-1}$ ) limited by temperature and solar radiation absorbed by the shaded and sunlit leaves. Since the WOFOST model considers the Green Area Index (GAI) emitted units, instead of leaves surface, both short- and long-term effects are computed each day for all the groups of emitted GAI units having the same age and then averaging the sum on the total number of contemporaneous age classes.

##### 4.4.2.1. Short-term response and ability of plant to recover from ozone damage

The short-term  $O_3$  effect on photosynthesis is computed daily for all GAI units of the same age class using a short-term hourly damage factor ( $GAI_{fO_{3,s(h)}}$ , 0 = maximum reduction; 1 = no effect; unit less) calculated, for each daylight hour, using a linear relationship between ozone uptake and the daily rate of gross photosynthesis (Equation 5; Figure 6; Ewert and Porter, 2000.).

$$GAI_{-fO_{3,s(h)}} = \begin{cases} 1 & \text{if } UO_{>FO3crit} \leq \frac{\gamma_1}{\gamma_2} \\ 1 - \gamma_1 - \gamma_2 UO_{>FO3crit} & \text{if } \frac{\gamma_1}{\gamma_2} < UO_{>FO3crit} < \frac{1 + \gamma_1}{\gamma_2} \\ 0 & \text{if } UO_{>FO3crit} \geq \frac{1 + \gamma_1}{\gamma_2} \end{cases} \quad [5]$$

Where:  $UO_{>FO3crit}$  ( $\text{nmol m}^{-2} \text{s}^{-1}$ ) is the instantaneous  $O_3$  leaf uptake rate (Equation 1);  $\gamma_1$  (unitless; default = 0.06) and  $\gamma_2$  ( $(\text{nmol m}^{-2} \text{s}^{-1})^{-1}$ ; default = 0.0045) represent short-term damage coefficients empirically determined.



**Figure 6. Relationship between factor accounting for short-term ozone effect on the daily rate of gross photosynthesis ( $GAI_{fO_{3,s(h)}}$ ) and ozone uptake.**

Hourly damage factors ( $GAI_{fO_{3,s(h)}}$ ) computed for daylight hours are then aggregated in a daily reduction factor ( $GAI_{fO_{3,s(d)}}$ ) for GAI units of the same age, considering both the damage caused by ozone during the previous hour ( $GAI_{fO_{3,s(h-1)}}$ ) and recovery from ozone injury of the previous day ( $GAI_{rO_{3,s}}$ ), as shown in Equation 6.

$$GAI_{-fO_{3,s(d)}} = \begin{cases} GAI_{-fO_{3,s(h)}} \cdot GAI_{-fO_{3,s(h-1)}} & \text{for } h = 1 + a..n + 1 \\ GAI_{-fO_{3,s(h)}} \cdot GAI_{rO_{3,s}} & \text{for } h = 1 \end{cases} \quad [6]$$

Where:  $a$  (h) is the first sunshine hour in the day;  $n$  (h) is the total number of sunshine hours in the day.

Since the plants are recovering from ozone damages of ozone during the night, the incomplete recovery from ozone damage ( $GAI_{rO_{3,s}}$ ) of the previous day is considered in the calculation of ozone effect on daily rates of  $CH_2O$  assimilation of the following day and it is dependent on leaf age (Equation 7; Figure 7).

$$GAI_{rO_{3,s}} = GAI_{-fO_{3,s(d-1)}} + (1 - GAI_{-fO_{3,s(d-1)}})GAI_{-f_{LA}} \quad [7]$$

Where:  $GAI_{f_{LA}}$  (1 = maximum recovery ability from ozone damage; 0 no recovery; unitless) is a factor accounting for leaf age and is computed over the life span of the GAI units.

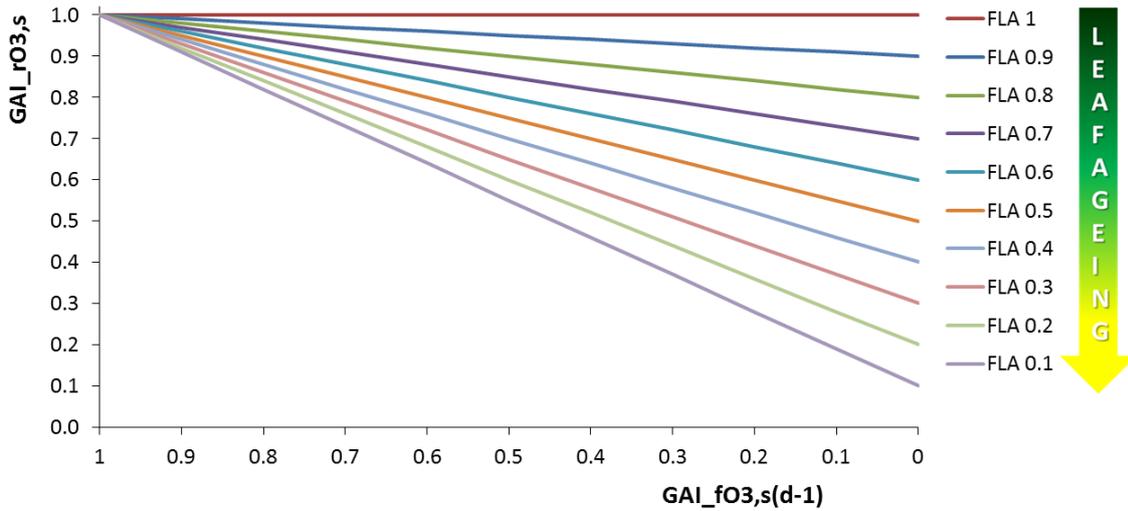
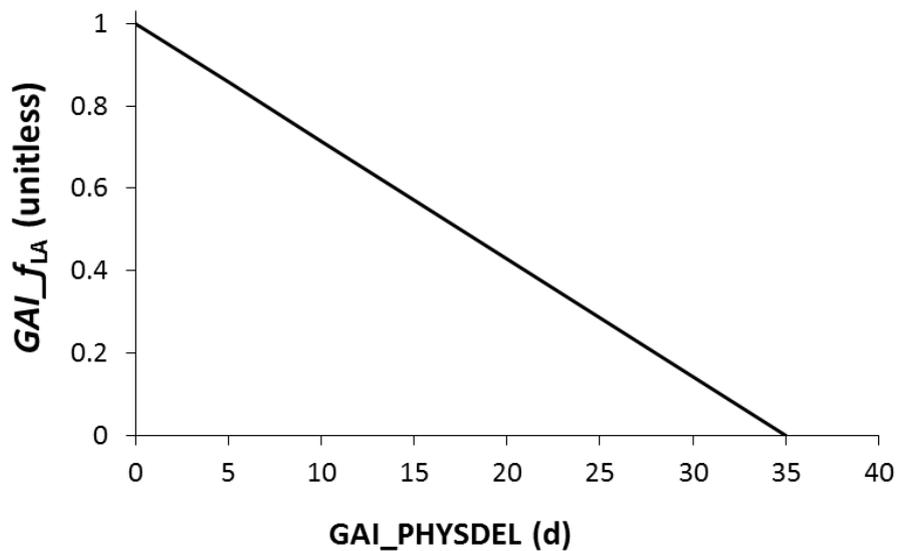


Figure 7. Recovery rates ozone injury factor ( $GAI_{rO_3,s}$ , unitless) as function of the short-term daily damage factors of the previous day ( $GAI_{fO_3,s(d-1)}$ , unitless) and leaf age ( $GAI_{f_{LA}}$ , unitless).

While young leaves can fully repair from  $O_3$  damage, the recover capacity decreases linearly with the ageing of the leaves up to zero when the leaf is dead (Equation 8; Figure 8).

$$GAI_{f_{LA}} = \begin{cases} 1 & \text{if } GAI_{PHYSDEL} = 0 \\ 1 - \frac{GAI_{PHYSDEL}}{GAI_{SPAN}} & \text{if } 0 < GAI_{PHYSDEL} < GAI_{SPAN} \\ 0 & \text{if } GAI_{PHYSDEL} \geq GAI_{SPAN} \end{cases} \quad [8]$$

Where:  $GAI_{PHYSDEL}$  (d) represents the physiological age of a representative leaf belonging to a given GAI unit;  $GAI_{SPAN}$  (d) is the life span of a representative leaf belonging to a given GAI unit.



**Figure 8. Relationship between factor used to simulate the recovery from ozone damage dependent on leaf age (GAI\_fLA) and the thermal life-span of a representative leaf belonging to a given GAI unit.**

An average short-term daily effect (Average\_GAI\_fO<sub>3,s(d)</sub>) is computed by averaging all daily reduction factors (GAI\_fO<sub>3,s(d)</sub>, specific for each contemporaneous GAI unit) and is then applied to reduce the gross photosynthesis rate calculated by WOFOST.

$$DGAR = DGAR \cdot \text{Average\_GAI\_fO}_{3,s(d)} \quad [9]$$

Where: DGAR (Kg ha<sup>-1</sup> d<sup>-1</sup>) represents the actual daily gross CH<sub>2</sub>O assimilation rate.

#### 4.4.2.2. Long-term response and acceleration of leaf senesce due to O<sub>3</sub> exposure

Both the signal for the onset of senescence and the rate of senescence are computed daily for each contemporaneous GAI unit using reducing factors (GAI\_fO<sub>3,l</sub>, 0 = maximum reduction; 1 = no effect; unit less) calculated as function of cumulative ozone uptake (Equation 10).

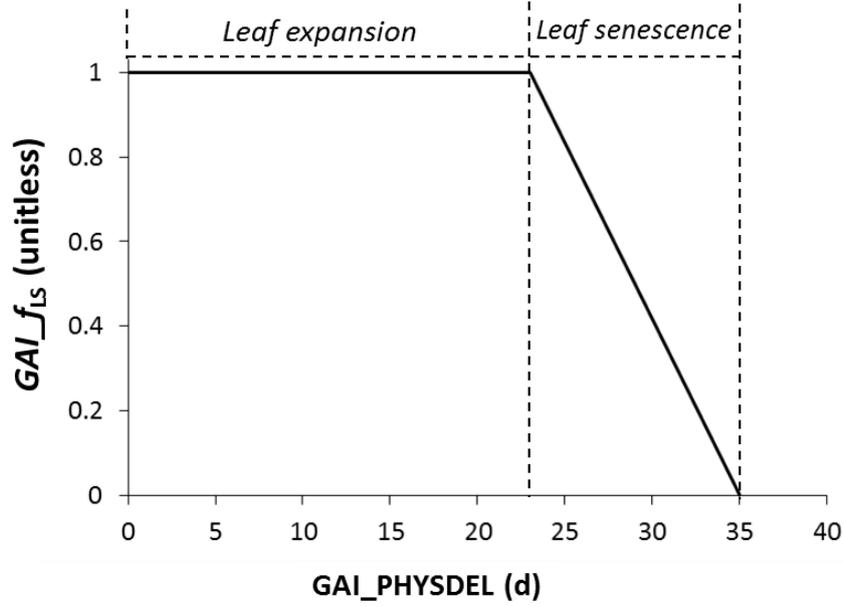
$$GAI\_fO_{3,l} = 1 - \gamma_3 \int_0^{t=GAI\_SPAN} \frac{UO_{>FO3crit}}{1000} \cdot h_{daylight} \quad [10]$$

Where:  $\gamma_3$  (( $\mu\text{mol m}^{-2}$ )<sup>-1</sup>; default = 0.5) is an ozone long-term damage coefficient, empirically determined, describing the reduction in the lifetime of a mature leaf per unit of ozone accumulated uptake;  $UO_{>FO3crit}$  (nmol m<sup>-2</sup> s<sup>-1</sup>) is the instantaneous O<sub>3</sub> leaf uptake rate (Equation 1);  $h_{daylight}$  (h) are the sunshine hours in a given day.

Then the factor accounting for the effect of leaf senescence on daily rate of gross photosynthesis (Figure 9) is calculated as,

$$GAI\_f_{LS} = \begin{cases} 1 & \text{if } GAI\_PHYSDEL \leq t_{l,ep} \\ \max \left[ \left[ 1 - \frac{GAI\_PHYSDEL - t_{l,ep}}{\frac{GAI\_SPAN}{GAI\_fO_{3,l}} - t_{l,ep}} \right], 0 \right] & \text{if } t_{l,ep} < GAI\_PHYSDEL < GAI\_SPAN \\ 0 & \text{if } GAI\_PHYSDEL \geq GAI\_SPAN \end{cases} \quad [11]$$

Where:  $t_{l,ep} = 0.33 \text{ GAI\_SPAN}$  (d) are the days during which a representative leaf belonging to a given GAI unit is fully expanded.



**Figure 9. Relationship between factor used to simulate the decline in the daily rate of gross photosynthesis in senescing leaves ( $GAI_{fLS}$ ) and the thermal life-span of a representative leaf belonging to a given GAI unit**

Finally, an average long-term daily effect ( $Average\_GAI_{fLS}$ ) is computed by averaging the sum of all daily reduction factor ( $GAI_{fLS}$ ) on the total number of contemporaneous age classes.

Since decreases in daily rate of gross photosynthesis are implicitly induced by the reduction in green leaf area indices (GAIs) daily associated to the faster ageing of each contemporaneous class of GAI units, the  $Average\_GAI_{fLS}$  factor is not applied to further reduce the actual daily gross  $CH_2O$  assimilation rate calculated by WOFOST in the modelling solution (Equation 9). The rationale for this is to reduce the risk of markedly overestimating the effect of senescence on reducing photosynthesis rates, double counting its impact on plant growth.

The effect of leaf senescence acceleration is computed daily in the ozone module by increasing the physiological age of all the contemporaneous GAI units ( $GAI\_PHYSDEL$ ) according to the Equation 12.

$$GAI\_PHYSDEL = GAI\_PHYSDEL_{(t-1)} + \max(GAI\_SPAN_{Adj(t-1)} - GAI\_SPAN_{Adj(t)}, 0) \quad [12]$$

Where:  $GAI\_SPAN_{Adj(t)}$  (d) is the life span of a given GAI unit modified by the ageing effect of cumulative ozone;  $GAI\_SPAN_{Adj(t-1)}$  (d) is the adjusted life span of the previous day.

Each day  $GAI\_SPAN_{Adj(t)}$  is calculated via Equation 13 and then used to update the WOFOST GAIage state variables of the following day.

$$GAI\_SPAN_{Adj(t)} = GAI\_SPAN_{Adj(t-1)} \cdot GAI_{fO3,l} \quad GAI\_SPAN_{Adj(t)} = GAI\_SPAN_{Adj(t-1)} \cdot GAI_{fO3,l} \quad [13]$$

The metacodes referring to the algorithms implemented for the short- and long-term effects are reported in Appendix B and C respectively.

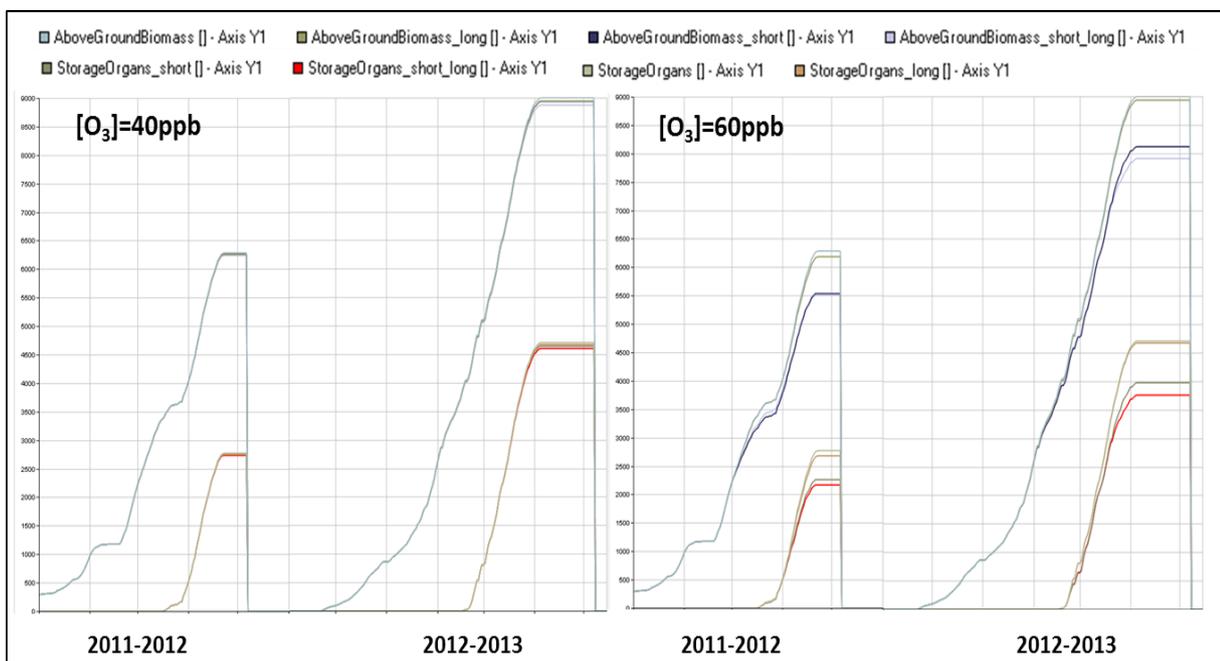
#### 4.5. Daily outputs

At the end of each simulation run, daily outputs of the CropML\_SoilW\_AbioticDamage\_solution are stored in .xls files and can be displayed via the Graphic Data Display (GDD) user interface application (<http://agsys.cra-cin.it/tools/gdd/help/>). Four different production levels are considered and results achieved for each of them are saved, separately in a dedicated sheet. This methodological choice allows to gain insight into the modeled effect of ozone damage on crop growth and productivity. The levels are:

- 1 **WL\_No O<sub>3</sub>**: it takes into account just water stress limitations to crop growth without considering any O<sub>3</sub> influence on crop phenology and productivity. Main daily outputs stored involve:
  - above ground biomass (AGB; Kg ha<sup>-1</sup>);
  - storage organs biomass (STO; Kg ha<sup>-1</sup>);
  - green lai index (GAI; m<sup>-2</sup> m<sup>-2</sup>);
  - soil water content (SWC; m<sup>-3</sup> m<sup>-3</sup>);
  - water stress index (WSI; unit less);
  - rooting depth (RD; m).
- 2 **WL\_O<sub>3</sub> Long**: it takes into account water stress limitations in conjunction with the O<sub>3</sub> long-term effect on crop growth and leaf senescence. Short-term O<sub>3</sub> effect is not considered. Main daily outputs stored involve:
  - AGB\_Long (Kg ha<sup>-1</sup>);
  - STO\_Long (Kg ha<sup>-1</sup>);
  - GAI\_Long (m<sup>-2</sup> m<sup>-2</sup>);
  - SWC\_Long (m<sup>-3</sup> m<sup>-3</sup>);
  - WSI\_Long (unit less);
  - RD\_Long (m);
  - O<sub>3</sub> flux to stomata (O<sub>3</sub>FluxTOSTomata\_Long; nmol m<sup>-2</sup> s<sup>-1</sup>);
  - Effect of water stress on stomatal conductance (Ks\_Long; unitless);
  - Percentage reduction of daily CH<sub>2</sub>O assimilation rate (%AssReduction\_Long; %).
- 3 **WL\_O<sub>3</sub> Short**: it takes into account water stress limitations in conjunction with the O<sub>3</sub> short-term effect on crop growth and leaf senescence. Long-term O<sub>3</sub> effect is not considered. Main daily outputs stored involve:
  - AGB\_Short (Kg ha<sup>-1</sup>);
  - STO\_Short (Kg ha<sup>-1</sup>);
  - GAI\_Short (m<sup>-2</sup> m<sup>-2</sup>);
  - SWC\_Short (m<sup>-3</sup> m<sup>-3</sup>);
  - WSI\_Short (unit less);
  - RD\_Short (m);
  - O<sub>3</sub>FluxTOSTomata\_Short (nmol m<sup>-2</sup> s<sup>-1</sup>);
  - Ks\_Short (unitless);
  - %AssReduction\_Short (%).
- 4 **WL\_O<sub>3</sub> Short x Long**: it takes into account water stress, long- and short-term O<sub>3</sub> limitations to growth and development. Main daily outputs stored involve:

- AGB\_Short x Long (Kg ha<sup>-1</sup>);
- STO\_Short x Long (Kg ha<sup>-1</sup>);
- GAI\_Short x Long (m<sup>-2</sup> m<sup>-2</sup>);
- SWC\_Short x Long (m<sup>-3</sup> m<sup>-3</sup>);
- WSI\_Short x Long (unit less);
- RD\_Short x Long (m);
- O<sub>3</sub>FluxTOSTomata\_Short x Long (nmol m<sup>-2</sup> s<sup>-1</sup>);
- Ks\_Short x Long (unitless);
- %AssReduction\_Short x Long (%).

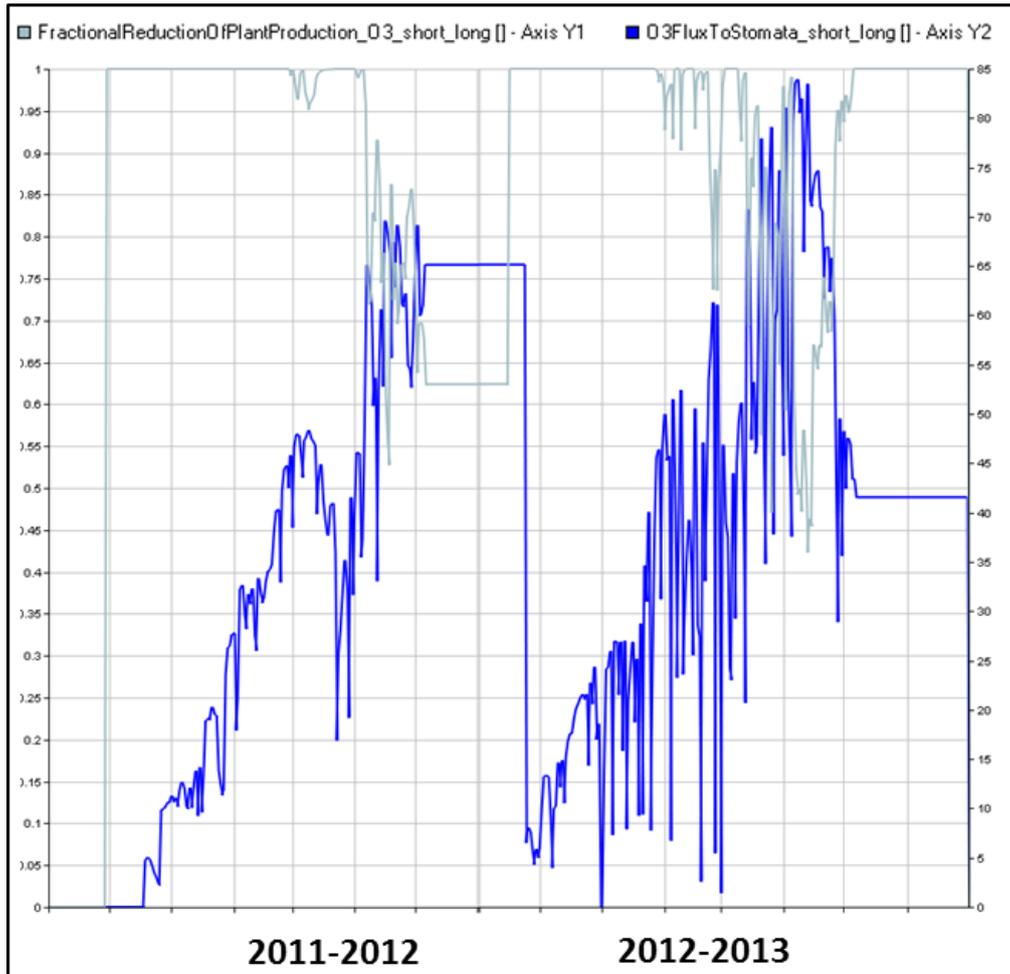
As an example, some results about the simulated impact of short- and long term O<sub>3</sub> exposure on wheat AGB and STO are presented in Figure 10, where two contrasting regimes of ozone concentration are compared.



**Figure 5. Graphic Data Display (GDD) interface showing aboveground biomass (kg ha<sup>-1</sup>) and storage organs biomass (kg ha<sup>-1</sup>) of wheat (water limited, Long-term O<sub>3</sub> limited, short term O<sub>3</sub> limited and with all limitations) simulated under two contrasting regimes of ozone concentration in a sample site of Northern Italy (seasons 2011-2012 and 2012-2013) with the CropML\_SoilW\_AbioticDamage\_solution.**

While crop productivity is slightly affected under the low-impact O<sub>3</sub> concentration regardless the production level considered, a decline in both AGB and STO up to -20:-25% is simulated under the enriched O<sub>3</sub> scenario, with differences depending on the variable and production level analyzed.

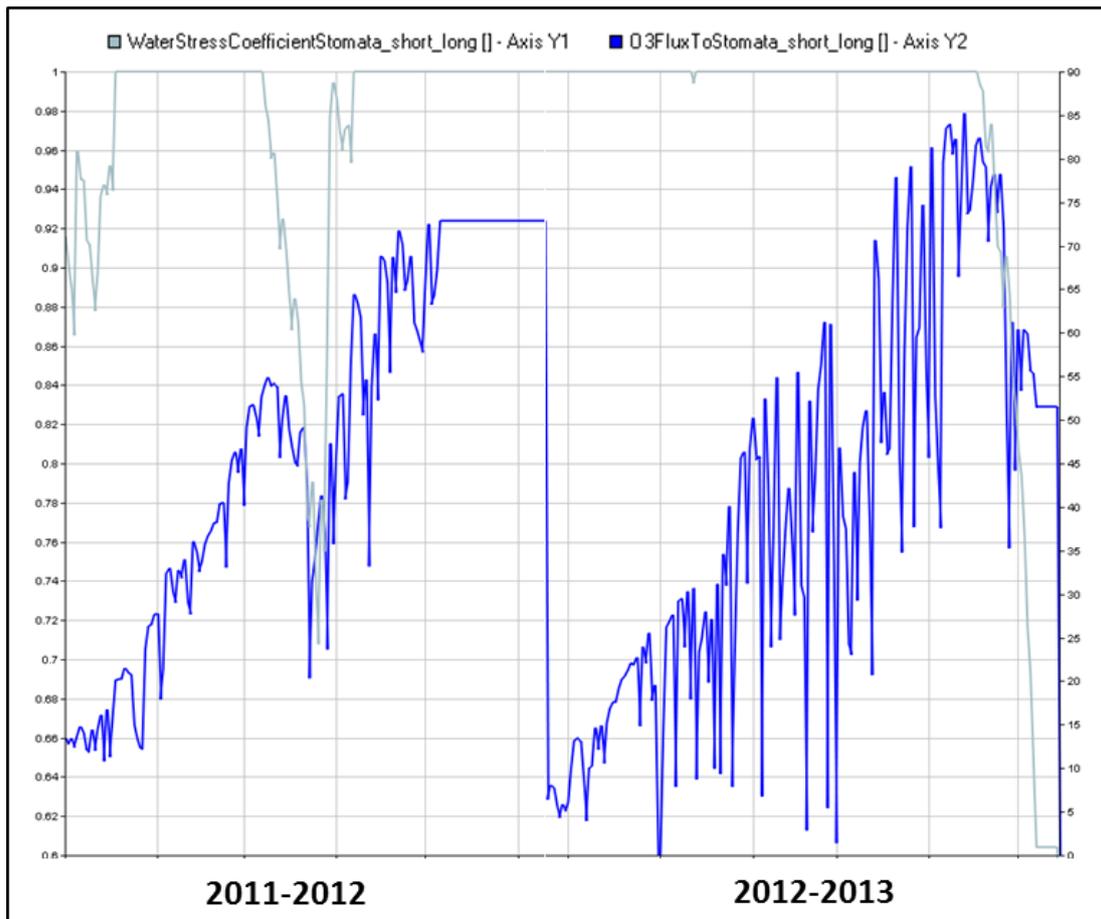
The percentage reduction of daily CH<sub>2</sub>O assimilation triggering the STO and AGB losses under the highest O<sub>3</sub> concentration are shown in Figure 11, where %AssReduction\_Short x Long data are plotted against O<sub>3</sub>FluxTOSTomata\_Short x long (nmol m<sup>-2</sup> s<sup>-1</sup>).



**Figure 6. Graphic Data Display (GDD) interface showing the percentage reduction of daily CH<sub>2</sub>O assimilation rate (%; light blue) against O<sub>3</sub> fluxes to stomata (nmol m<sup>-2</sup> s<sup>-1</sup>; blue) simulated under enriched O<sub>3</sub> concentration (60 ppb) for the limited production level (seasons 2011-2012 and 2012-2013).**

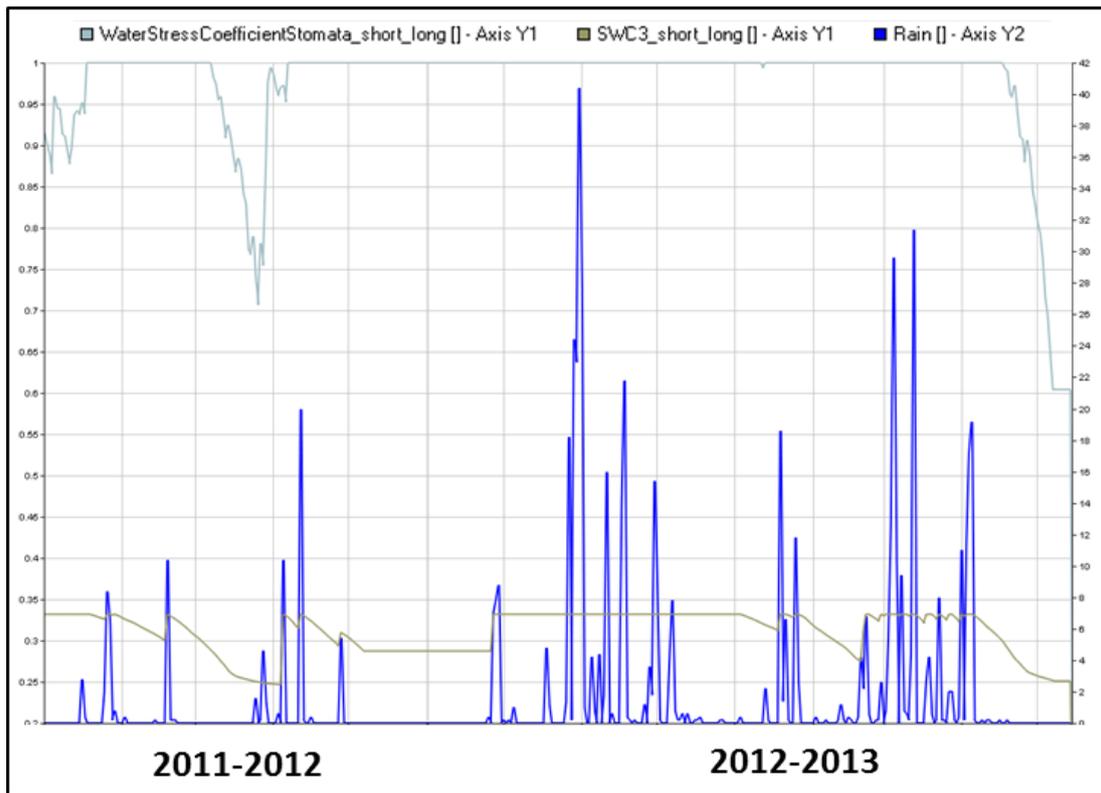
As it can be noticed, O<sub>3</sub> fluxes to stomata frequently exceeded a threshold for damage in the growing season 2012-2013 causing decreases in daily assimilation rate up to 60 %, whereas in 2011-2012 reductions in assimilation rates were mainly confined toward the end of the season. Daily fluctuations in O<sub>3</sub> fluxes to stomata strictly depend on aerodynamic boundary layer resistance and stomatal conductivity, as influenced by intercepted solar radiation, O<sub>3</sub> effect and water stress.

A picture of the effect of water stress on stomatal conductivity and its relationships with O<sub>3</sub> fluxes to stomata are shown in Figure 12.



**Figure 7. Graphic Data Display (GDD) interface showing the effect of water stress on stomatal conductance ( $Ks\_Long$ ; unitless; light blue)  $O_3$  fluxes to stomata ( $nmol\ m^{-2}\ s^{-1}$ ; blue) simulated under enriched  $O_3$  concentration (60 ppb) for the all limited production level (seasons 2011-2012 and 2012-2013).**

The water stress-induced reduction of stomatal conductance simulated in the first part of the season largely contributed to protect the crop from  $O_3$  damage in 2011-2012, whereas in the following season the crop had less benefit from this mechanism, due to the higher amount of rainfall and soil water content in the rooted zone (Figure 13).



**Figure 8. Graphic Data Display (GDD) interface showing the effect of water stress on stomatal conductance ( $Ks\_Long$ ; unitless; light blue), daily rainfall patterns (mm) and the soil water content in the rooted zone (mm) simulated under enriched  $O_3$  concentration (60 ppb) for the all limited production level (seasons 2011-2012 and 2012-2013).**

To conclude, a synthetic overview of possible fluctuations of  $O_3$  fluxes to stomata and of percentage reduction of daily  $CH_2O$  assimilation rate as function of the variation of ozone short-term damage coefficients  $\gamma_1$  and  $\gamma_2$ . (Equation 5) are shown in Figure 14; the flux of  $90 \text{ nmol m}^{-2} \text{ s}^{-1}$  was selected since coherent with those simulated in figure 13 and 14.

Flux to stomata ( $nmol\ m^{-2}\ s^{-1}$ )

$v_2/v_1$	0.05	0.1	0.15	0.2	0.25	0.3	0.35	0.4	0.45	0.5	0.55	0.6	0.65	0.7	0.75	0.8	0.85	0.9	0.95	1
0.0005	100	200	300	400	500	600	700	800	900	1000	1100	1200	1300	1400	1500	1600	1700	1800	1900	2000
0.001	50	100	150	200	250	300	350	400	450	500	550	600	650	700	750	800	850	900	950	1000
0.0015	33.3333	66.6667	100	133.3333	166.6667	200	233.3333	266.6667	300	333.3333	366.6667	400	433.3333	466.6667	500	533.3333	566.6667	600	633.3333	666.6667
0.002	25	50	75	100	125	150	175	200	225	250	275	300	325	350	375	400	425	450	475	500
0.0025	20	40	60	80	100	120	140	160	180	200	220	240	260	280	300	320	340	360	380	400
0.003	16.6667	33.3333	50	66.6667	83.3333	100	116.6667	133.3333	150	166.6667	183.3333	200	216.6667	233.3333	250	266.6667	283.3333	300	316.6667	333.3333
0.0035	14.2857	28.5714	42.8571	57.1428	71.4286	85.7143	100	114.2857	128.5714	142.8571	157.1429	171.4286	185.7143	200	214.2857	228.5714	242.8571	257.1429	271.4286	285.7143
0.004	12.5	25	37.5	50	62.5	75	87.5	100	112.5	125	137.5	150	162.5	175	187.5	200	212.5	225	237.5	250
0.0045	11.1111	22.2222	33.3333	44.4444	55.5556	66.6667	77.7778	88.8889	100	111.1111	122.2222	133.3333	144.4444	155.5556	166.6667	177.7778	188.8889	200	211.1111	222.2222
0.005	10	20	30	40	50	60	70	80	90	100	110	120	130	140	150	160	170	180	190	200
0.0055	9.0909	18.1818	27.2727	36.3636	45.4545	54.5455	63.6364	72.7273	81.8182	90.9091	100	109.0909	118.1818	127.2727	136.3636	145.4545	154.5455	163.6364	172.7273	181.8182
0.006	8.3333	16.6667	25	33.3333	41.6667	50	58.3333	66.6667	75	83.3333	91.6667	100	108.3333	116.6667	125	133.3333	141.6667	150	158.3333	166.6667
0.0065	7.6923	15.3846	23.0769	30.7692	38.4615	46.1538	53.8462	61.5385	69.2308	76.9231	84.6154	92.3077	100	107.6923	115.3846	123.0769	130.7692	138.4615	146.1538	153.8462
0.007	7.1428	14.2857	21.4286	28.5714	35.7143	42.8571	50	57.1429	64.2857	71.4286	78.5714	85.7143	92.8571	100	107.1429	114.2857	121.4286	128.5714	135.7143	142.8571
0.0075	6.6667	13.3333	20	26.6667	33.3333	40	46.6667	53.3333	60	66.6667	73.3333	80	86.6667	93.3333	100	106.6667	113.3333	120	126.6667	133.3333
0.008	6.25	12.5	18.75	25	31.25	37.5	43.75	50	56.25	62.5	68.75	75	81.25	87.5	93.75	100	106.25	112.5	118.75	125
0.0085	5.8824	11.7647	17.6471	23.5294	29.4118	35.2941	41.1765	47.0588	52.9412	58.8235	64.7059	70.5882	76.4706	82.3529	88.2353	94.1177	100	105.8824	111.7647	117.6471
0.009	5.5556	11.1111	16.6667	22.2222	27.7778	33.3333	38.8889	44.4444	50	55.5556	61.1111	66.6667	72.2222	77.7778	83.3333	88.8889	94.4444	100	105.5556	111.1111
0.0095	5.2632	10.5263	15.7895	21.0526	26.3158	31.5789	36.8421	42.1053	47.3684	52.6316	57.8947	63.1579	68.4211	73.6842	78.9474	84.2106	89.4737	94.7369	100	105.2632
0.01	5	10	15	20	25	30	35	40	45	50	55	60	65	70	75	80	85	90	95	100

Daily assimilation rate reduction ( $1=no\ impact; 0=max\ impact; unitless$ ) at a flux of  $90\ nmol\ m^{-2}$

$v_2/v_1$	0.05	0.1	0.15	0.2	0.25	0.3	0.35	0.4	0.45	0.5	0.55	0.6	0.65	0.7	0.75	0.8	0.85	0.9	0.95	1
0.0005	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
0.001	0.96	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
0.0015	0.915	0.965	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
0.002	0.87	0.92	0.97	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
0.0025	0.825	0.875	0.925	0.975	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
0.003	0.78	0.83	0.88	0.93	0.98	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
0.0035	0.735	0.785	0.835	0.885	0.935	0.985	1	1	1	1	1	1	1	1	1	1	1	1	1	1
0.004	0.69	0.74	0.79	0.84	0.89	0.94	0.99	1	1	1	1	1	1	1	1	1	1	1	1	1
0.0045	0.645	0.695	0.745	0.795	0.845	0.895	0.945	0.995	1	1	1	1	1	1	1	1	1	1	1	1
0.005	0.6	0.65	0.7	0.75	0.8	0.85	0.9	0.95	1	1	1	1	1	1	1	1	1	1	1	1
0.0055	0.555	0.605	0.655	0.705	0.755	0.805	0.855	0.905	0.955	1	1	1	1	1	1	1	1	1	1	1
0.006	0.51	0.56	0.61	0.66	0.71	0.76	0.81	0.86	0.91	0.96	1	1	1	1	1	1	1	1	1	1
0.0065	0.465	0.515	0.565	0.615	0.665	0.715	0.765	0.815	0.865	0.915	0.965	1	1	1	1	1	1	1	1	1
0.007	0.42	0.47	0.52	0.57	0.62	0.67	0.72	0.77	0.82	0.87	0.92	0.97	1	1	1	1	1	1	1	1
0.0075	0.375	0.425	0.475	0.525	0.575	0.625	0.675	0.725	0.775	0.825	0.875	0.925	0.975	1	1	1	1	1	1	1
0.008	0.33	0.38	0.43	0.48	0.53	0.58	0.63	0.68	0.73	0.78	0.83	0.88	0.93	0.98	1	1	1	1	1	1
0.0085	0.285	0.335	0.385	0.435	0.485	0.535	0.585	0.635	0.685	0.735	0.785	0.835	0.885	0.935	0.985	1	1	1	1	1
0.009	0.24	0.29	0.34	0.39	0.44	0.49	0.54	0.59	0.64	0.69	0.74	0.79	0.84	0.89	0.94	0.99	1	1	1	1
0.0095	0.195	0.245	0.295	0.345	0.395	0.445	0.495	0.545	0.595	0.645	0.695	0.745	0.795	0.845	0.895	0.945	0.995	1	1	1
0.01	0.15	0.2	0.25	0.3	0.35	0.4	0.45	0.5	0.55	0.6	0.65	0.7	0.75	0.8	0.85	0.9	0.95	1	1	1

Figure 9. Changes in the values of  $O_3$  flux to stomata ( $nmol\ m^{-2}\ s^{-1}$ ) and in the factor triggering the reduction of daily  $CH_2O$  assimilation rate (%) as function of different combinations of short-term damage coefficients  $v_1$  and  $v_2$

## 5. Preliminary results from the test conditions experiment

The preliminary results of the simulations to evaluate the sensitivity of the modelling solution to ozone exposure under the test conditions described in section 3 are reported below as:

- boxplots, to show the variability in the 20-years series of simulated outputs;
- daily dynamics, to highlight the differences in model behavior in contrasting growing seasons (e.g. high versus low impact years).

We note here, that the evaluation of the model results against observations, would need the evaluation of detailed chamber and field studies in a coherent way, which will be performed in different study.

While the seasonal outputs aim to highlight the differences among the short-, long- and short&long production levels (as explained in section 4.5) and the consecutive impacts of O<sub>3</sub> damage on yield, the long-term simulations refer exclusively to the Short & Long production level and concern:

- final AGB (kg ha<sup>-1</sup>), final yield (kg ha<sup>-1</sup>) and maximum green leaf area index (m<sup>2</sup> m<sup>-2</sup>) among the growth variables,
- number of days with O<sub>3</sub> flux exceeding the critical crop-specific O<sub>3</sub> concentration (d), average fractional reduction of daily gross CH<sub>2</sub>O assimilation rate during the crop cycle (%), the cumulative O<sub>3</sub> fluxes during the growing season (nmol m<sup>-2</sup>) among the variables triggering the O<sub>3</sub> damages.

### 5.1. Long-term simulations under different tropospheric O<sub>3</sub> concentrations

Figures 15-18, show yields for wheat and barley in Bremen and Jerez for different ozone conditions: 20 ppb (pre-industrial), 40 ppb (current background), and 60 ppb (polluted), the latter average over the growing season, or in specific months on top of the 40 ppb background conditions. Irrespective of ozone, rainfed wheat and barley yields are lower by only 12 % in Bremen compared to fully irrigated crops, while strongly reduced by 55 % in Jerez. Additionally, wheat yield losses, up to 30 % are calculated for ozone concentrations of 60 ppb, and only half of these for barley. Yield losses are substantially smaller in Jerez for rain-fed crops, when stomatal closure is limiting gas exchange, and thus impeding photosynthesis, crop growth and yields, but also reducing ozone uptake.

### 5.1.1. Final Yield

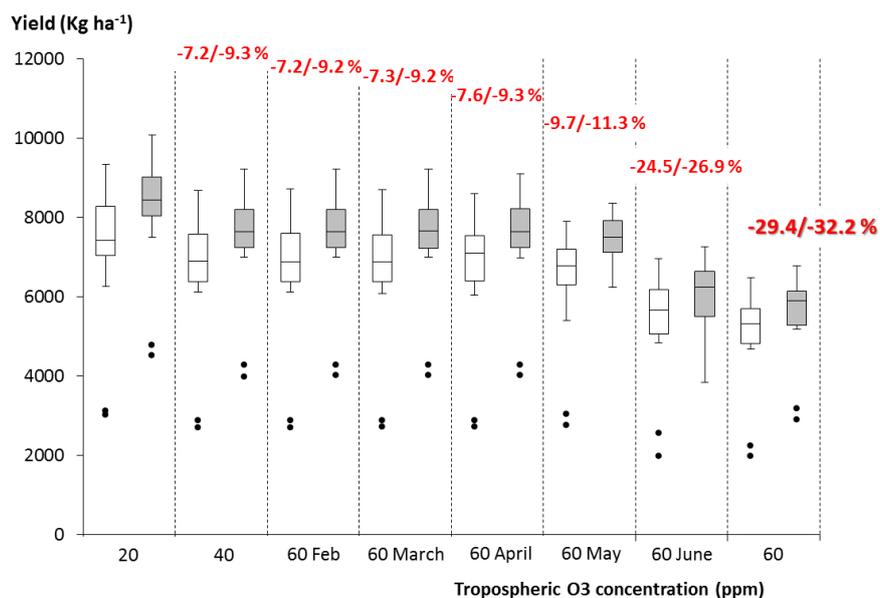


Figure 10. Boxplot of final yield values (kg ha<sup>-1</sup>) simulated for the pre-industrial, background and high ozone concentrations scenarios. Each box is derived from the 19 annual values simulated for wheat crop in Bremen, Germany. Open boxes refer to rainfed; grey boxes to fully irrigated conditions. Dots represent results for the two lowest extreme years. Red numbers represent the relative reduction due to ozone compared to the 20 ppb case.

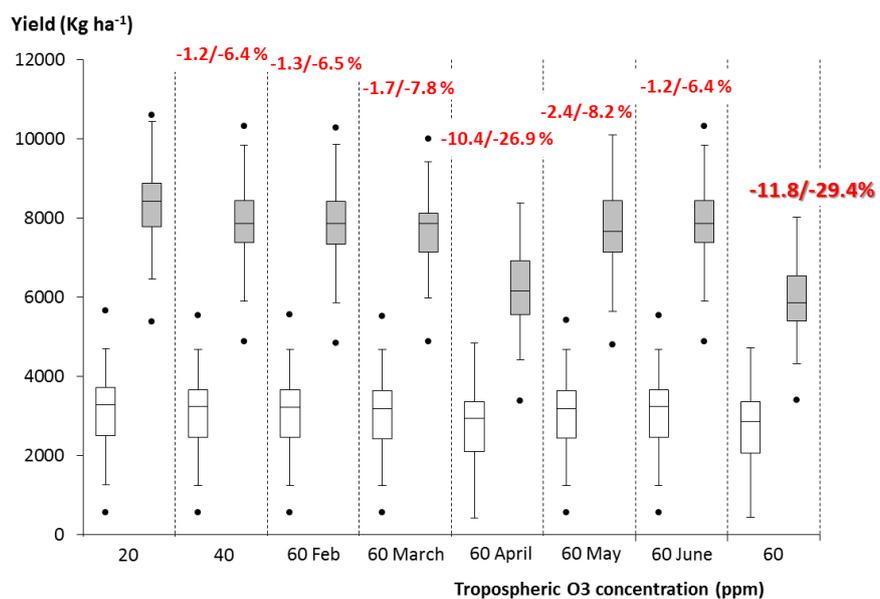


Figure 11. Boxplot of final yield values (kg ha<sup>-1</sup>) simulated for the pre-industrial, background and high ozone concentrations scenarios. Each box is derived from the 19 values simulated for wheat crop in Jerez de la Frontera, Spain. Open boxes refer to rainfed conditions, grey boxes to fully irrigated conditions. Dots represent results for the two lowest extreme years. Red numbers represent the relative reduction due to ozone compared to the 20 ppb case.

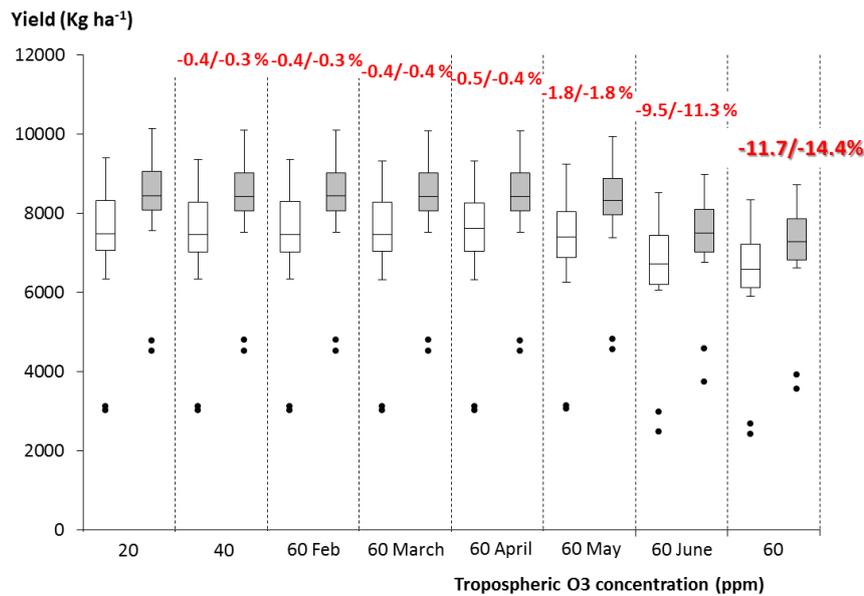


Figure 17. Boxplot of final yield values (Kg ha<sup>-1</sup>) simulated for the pre-industrial, back ground and high Ozone concentrations scenarios. Each box is derived from the 19 values simulated for **barley** crop in Bremen, Germany. Open boxes refer to rainfed conditions, grey boxes to fully irrigated conditions. Dots represent results for the two lowest extreme years. Red numbers represent the relative reduction due to ozone compared to the 20 ppb case.

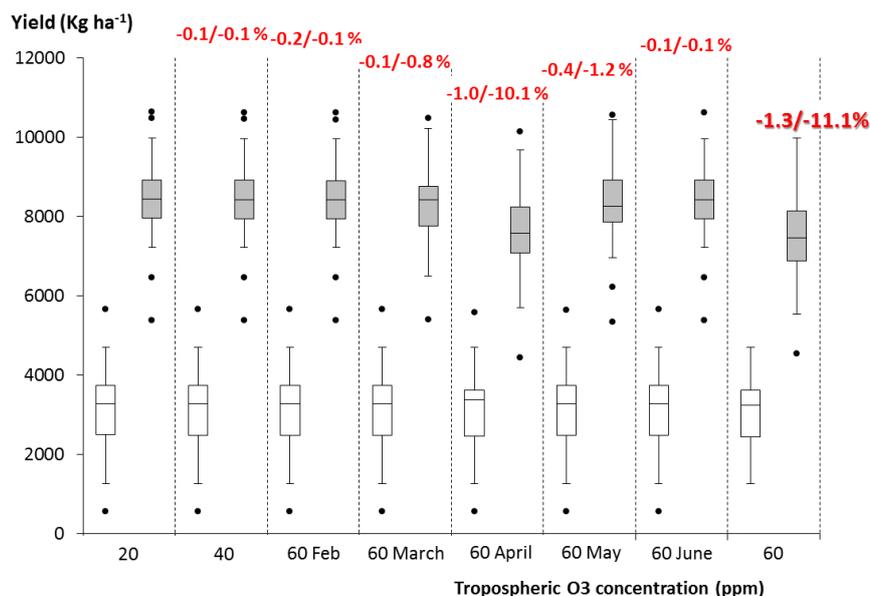
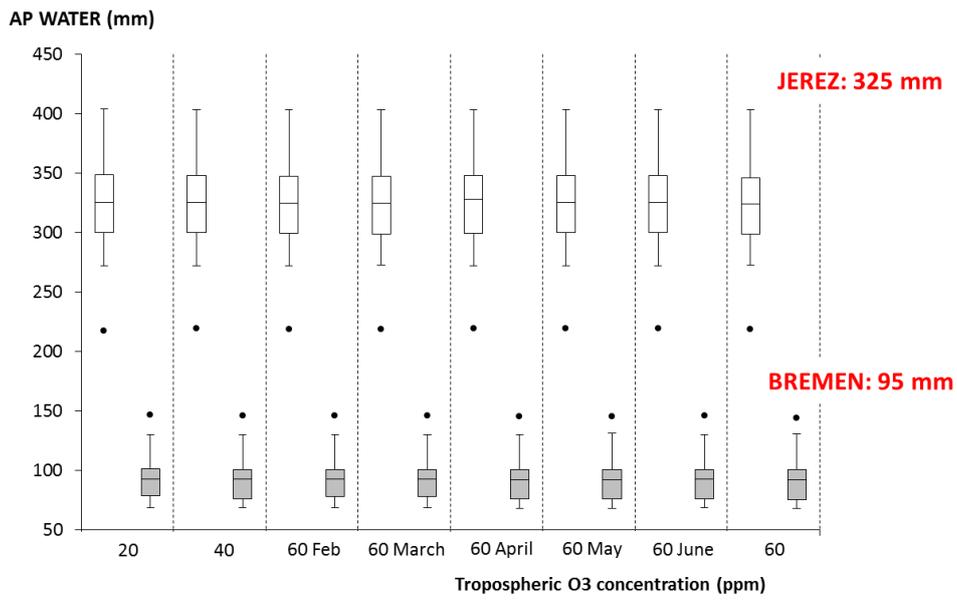


Figure 18. Boxplot of final yield values (kg ha<sup>-1</sup>) simulated for the pre-industrial (20 ppb), back ground (40 ppb) and high (60 ppb) Ozone concentrations scenarios. Each box is derived from the 19 values simulated for barley crop in Jerez de la Frontera, Spain. Open boxes refer to rainfed conditions, grey boxes to fully irrigated conditions. Dots represent results for the two lowest extreme years. Red numbers represent the relative reduction due to ozone compared to the 20 ppb case.

Figure 19 shows that despite different ozone impacts on crop, the ‘fully irrigated’ water use was not strongly affected.



**Figure 19. Boxplot of absolute amounts of water (mm) applied to wheat/barley crops during the growing seasons under the fully irrigated conditions for the pre-industrial, back ground and high Ozone concentrations scenarios. Each box is derived from the 19 values simulated for barley crop in Jerez de la Frontera, Spain. Open boxes refer Bremen, grey boxes to Jerez de la Frontera.**

### 5.1.2. Final above ground biomass (AGB)

Figure 20-23 demonstrate that in relative terms the amount of biomass at harvest was similar to yield decline, in relative terms. Absolute biomass loss was much higher in Jerez compared to Bremen, but the relative losses were smaller in Jerez due to stomatal closure under hot conditions. Biomass losses in Barley were less than in wheat.

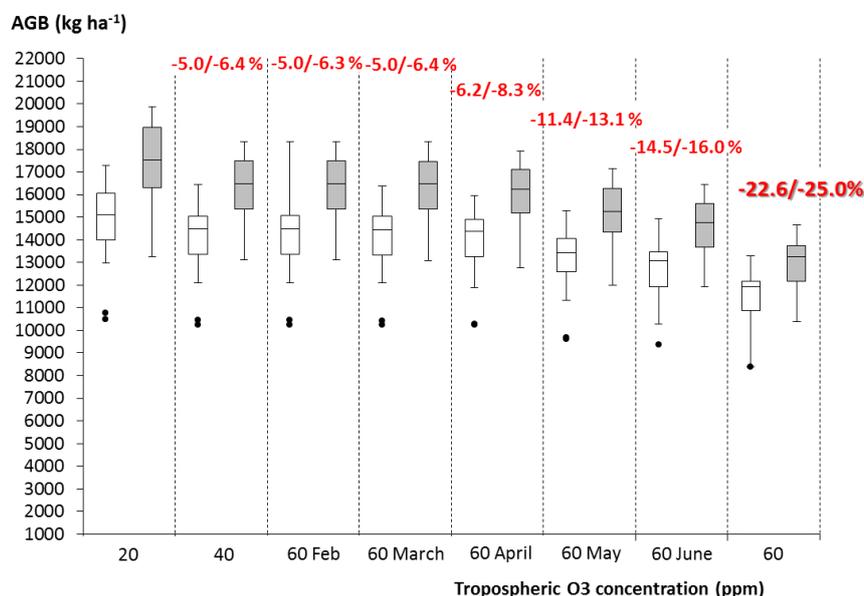


Figure 12. Boxplot of final AGB (Kg ha<sup>-1</sup>) simulated for the pre-industrial, back ground and high Ozone concentrations scenarios. Each box is derived from the 19 values simulated for wheat crop in Bremen, Germany. Open boxes refer to rainfed conditions, grey boxes to fully irrigated conditions.

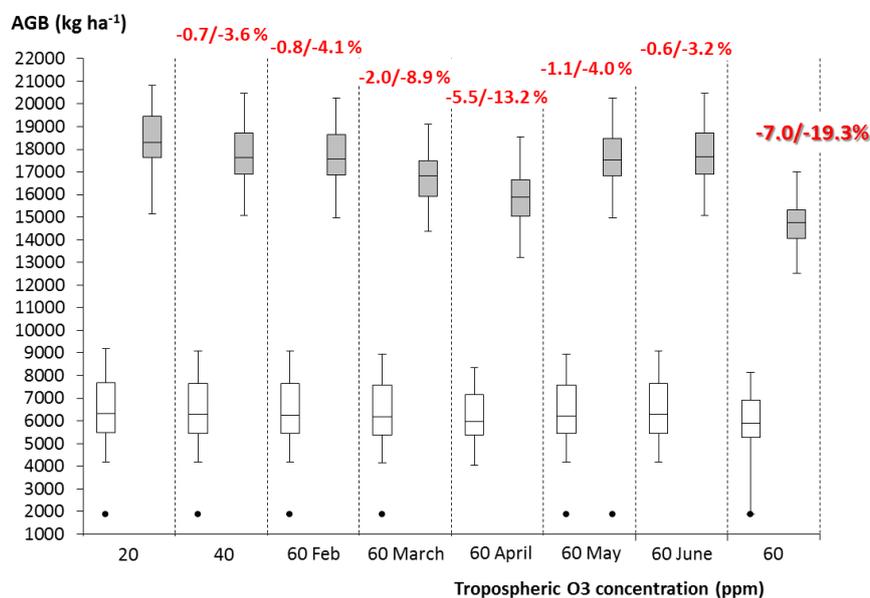


Figure 13. Boxplot of final AGB (kg ha<sup>-1</sup>) simulated for the pre-industrial, back ground and high Ozone concentrations scenarios. Each box is derived from the 19 values simulated for wheat crop in Jerez de la Frontera, Spain. Open boxes refer to rainfed conditions, grey boxes to fully irrigated conditions.

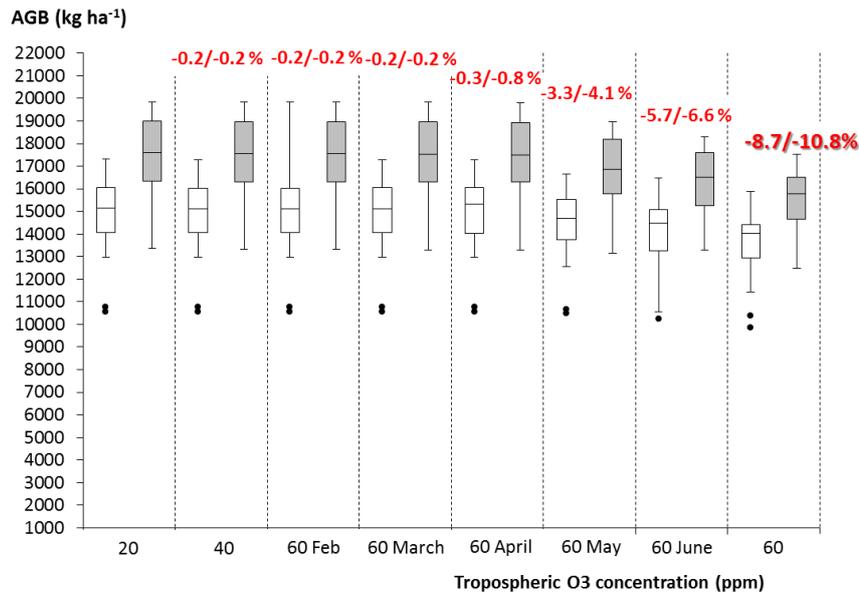


Figure 14. Boxplot of final AGB (kg ha<sup>-1</sup>) simulated for the pre-industrial, back ground and high Ozone concentrations scenarios. Each box is derived from the 19 values simulated for barley crop in Bremen, Germany. Open boxes refer to rainfed conditions, grey boxes to fully irrigated conditions.

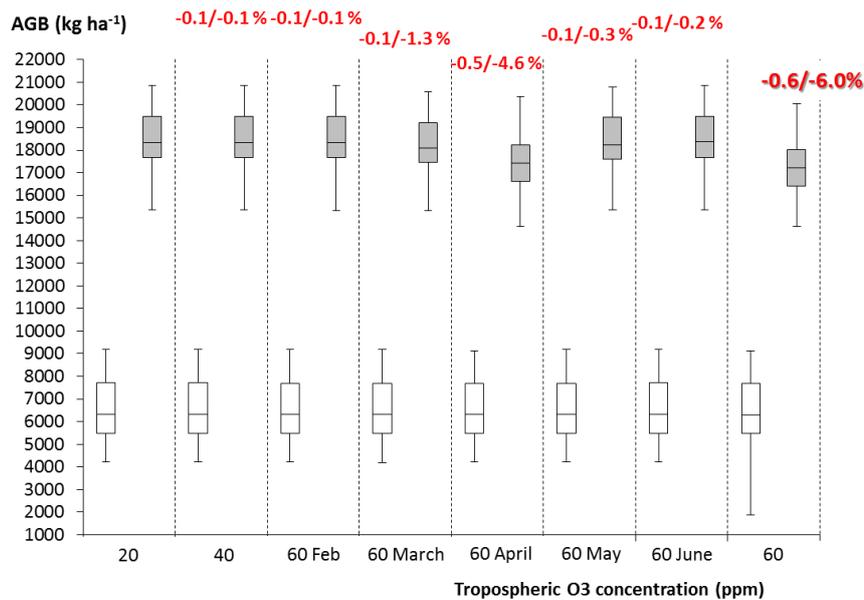


Figure 15. Boxplot of AGB (kg ha<sup>-1</sup>) simulated for the pre-industrial, back ground and high Ozone concentrations scenarios. Each box is derived from the 19 values simulated for barley crop in Jerez de la Frontera, Spain. Open boxes refer to rainfed conditions, grey boxes to fully irrigated conditions.

### 5.1.3. Maximum green leaf area index (GLAI<sub>max</sub>)

The green leaf area ( $m^2$ ) divided by the ground area ( $m^2$ ) GLAI (Figure 24-27) is an indicator for crop growth, and is usually maximizing around flowering. GLAI values are in a realistic range for all ozone cases (wheat/barley), and show substantially lower declines than biomass, indicating to a substantial amount of assimilates used for respiration/repair.

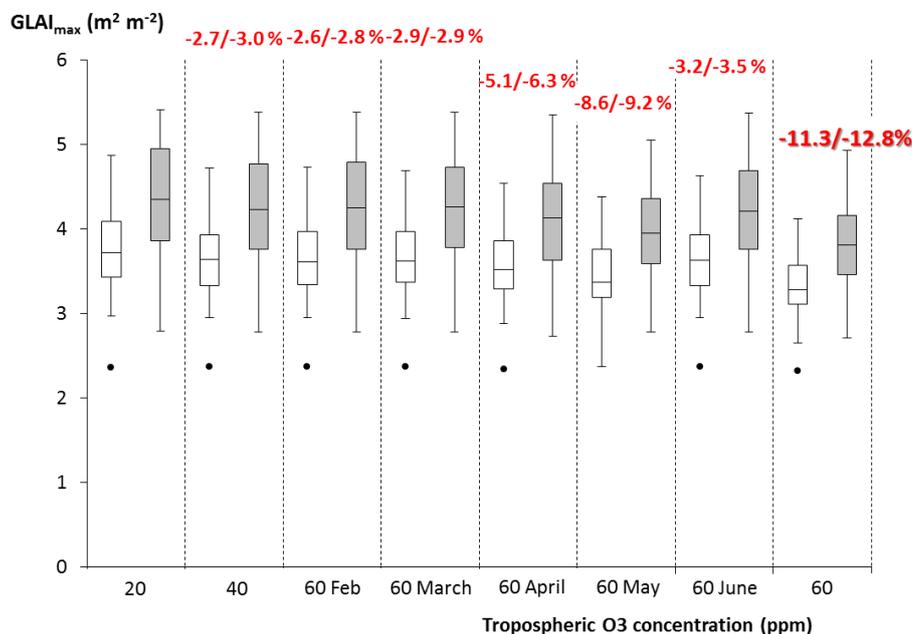


Figure 16. Boxplot of maximum GLAI ( $m^2 m^{-2}$ ) simulated for the pre-industrial, back ground and high ozone concentrations scenarios. Each box is derived from the 19 values simulated for wheat crop in Bremen, Germany. Open boxes refer to rainfed conditions, grey boxes to fully irrigated conditions.

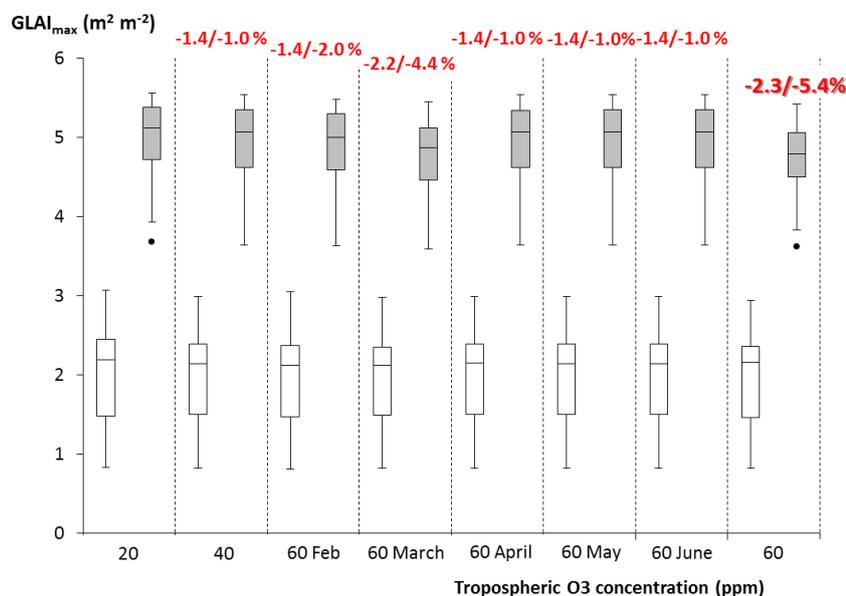


Figure 17. Boxplot of maximum GLAI ( $m^2 m^{-2}$ ) simulated for the pre-industrial, back ground and high Ozone concentrations scenarios. Each box is derived from the 19 values simulated for wheat crop in Jerez de la Frontera, Spain. Open boxes refer to rainfed conditions, grey boxes to fully irrigated conditions.

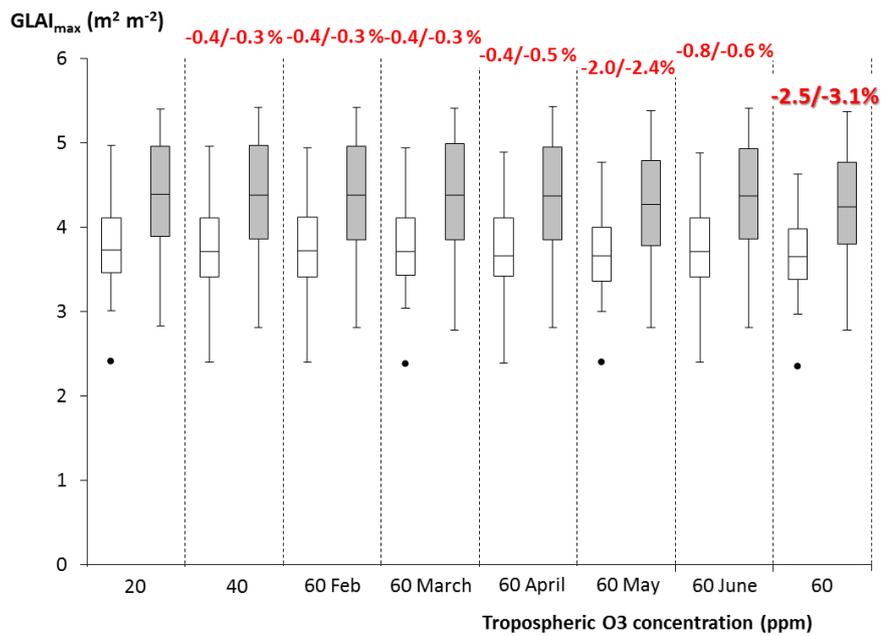


Figure 18. Boxplot of maximum GLAI ( $\text{m}^2 \text{m}^{-2}$ ) simulated for the pre-industrial, back ground and high Ozone concentrations scenarios. Each box is derived from the 19 values simulated for barley crop in Bremen, Germany. Open boxes refer to rainfed conditions, grey boxes to fully irrigated conditions.

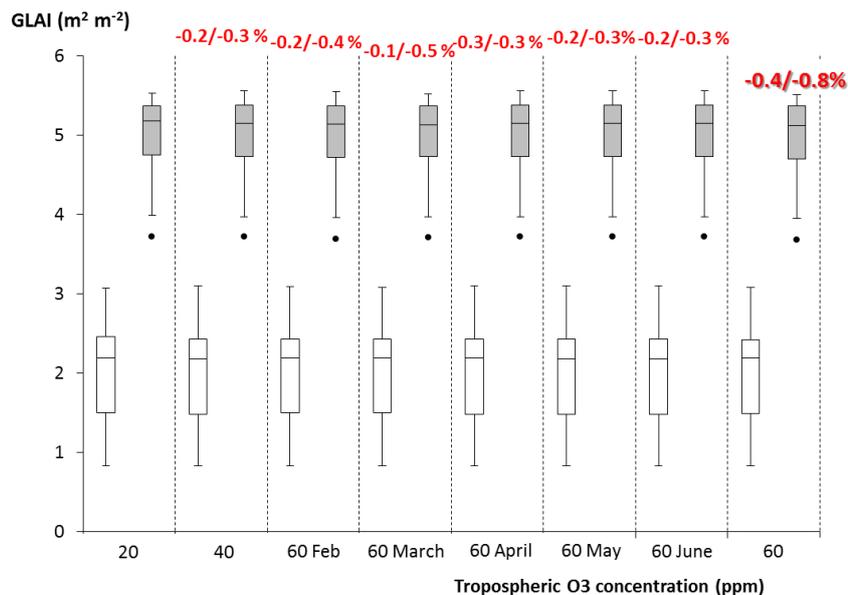


Figure 27. Boxplot of maximum GLAI ( $\text{m}^2 \text{m}^{-2}$ ) simulated for the pre-industrial, back ground and high Ozone concentrations scenarios. Each box is derived from the 19 values simulated for barley crop in Jerez de la Frontera, Spain. Open boxes refer to rainfed conditions, grey boxes to fully irrigated conditions.

### 5.1.4. Days with O<sub>3</sub> flux exceeding the critical O<sub>3</sub> concentration (O<sub>3</sub> flux > O<sub>3crit</sub>)

Figure 28-31 show the number of days where the O<sub>3</sub> flux is exceeding the critical thresholds, see section 4.4.2.1. Elevated (60 ppb) ozone adds approximately 5-10 additional days each month above the threshold flux, summing to 50 additional days at harvest in Bremen for wheat. At Jerez, under water limited conditions the number of days above critical ozone fluxes is quite limited, but more pronounced under irrigated conditions.

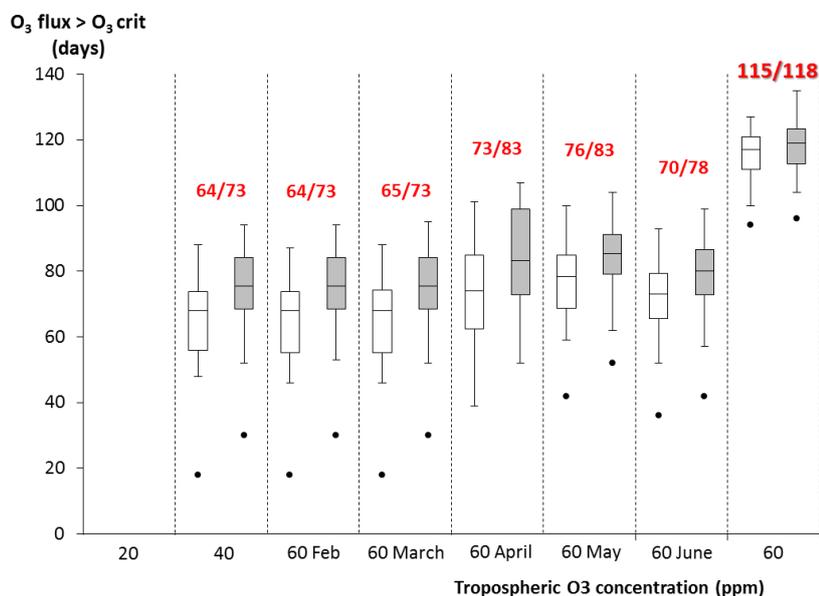


Figure 28. Boxplot of number of days with O<sub>3</sub> flux > O<sub>3</sub> crit. (days) simulated for the pre-industrial, back ground and high Ozone concentrations scenarios. Each box is derived from the 19 values simulated for wheat crop in Bremen, Germany. Open boxes refer to rainfed conditions, grey boxes to fully irrigated conditions.

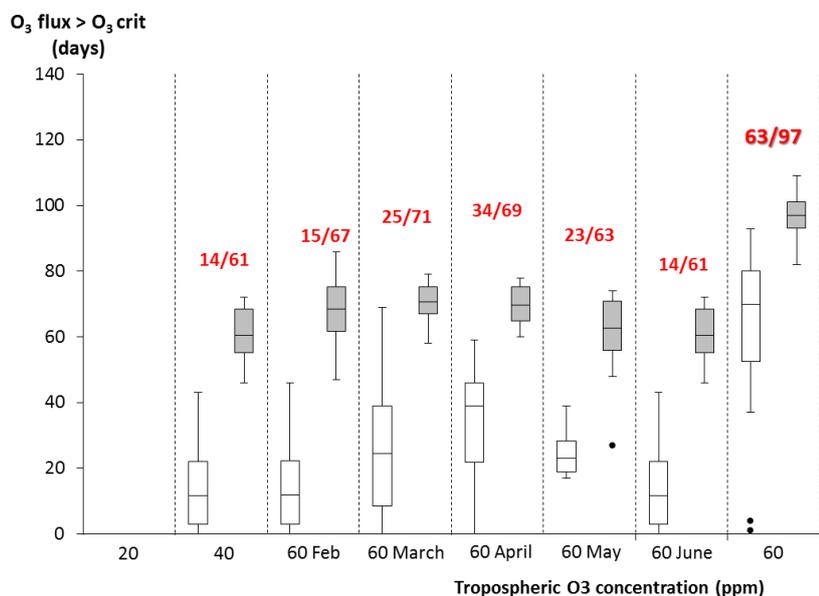


Figure 29. Boxplot of number of days with O<sub>3</sub> flux > O<sub>3</sub> crit. (days) simulated for the pre-industrial, back ground and high Ozone concentrations scenarios. Each box is derived from the 19 values simulated for wheat crop in Jerez de la Frontera, Spain. Open boxes refer to rainfed conditions, grey boxes to fully irrigated conditions.

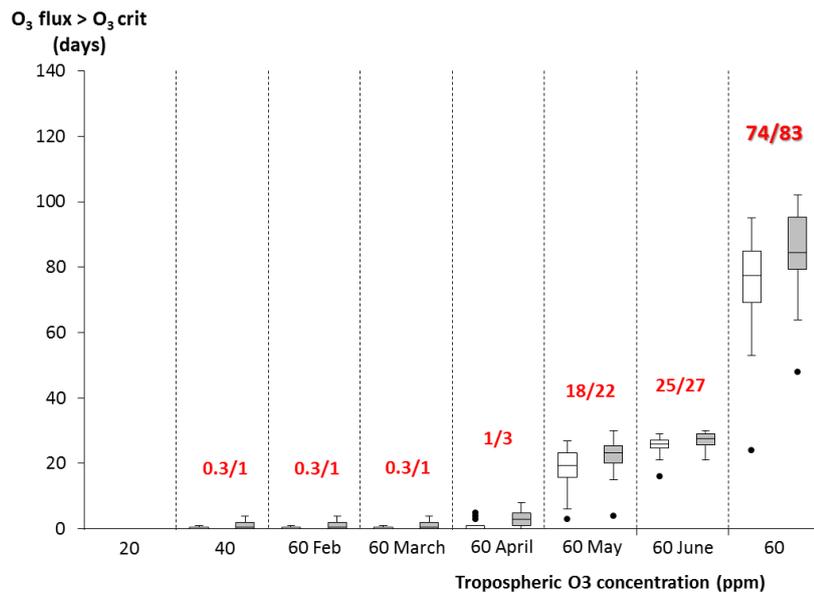


Figure 19. Boxplot of number of days with  $O_3$  flux  $>$   $O_3$  crit. (days) simulated for the pre-industrial, back ground and high Ozone concentrations scenarios. Each box is derived from the 19 values simulated for barley crop in Bremen, Germany. Open boxes refer to rainfed conditions, grey boxes to fully irrigated conditions.

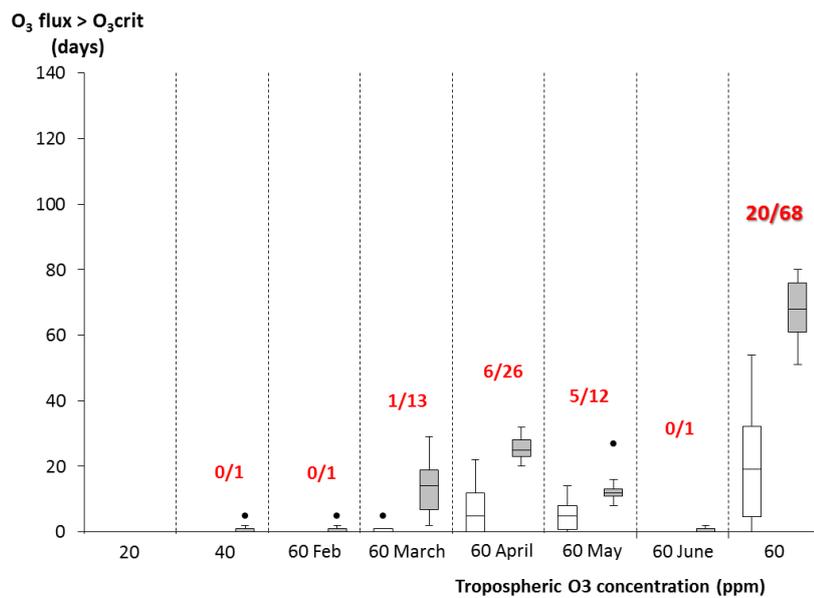


Figure 20. Boxplot of number of days with  $O_3$  flux  $>$   $O_3$  crit. (days) simulated for the pre-industrial, back ground and high Ozone concentrations scenarios. Each box is derived from the 19 values simulated for barley crop in Jerez de la Frontera, Spain. Open boxes refer to rainfed conditions, grey boxes to fully irrigated conditions.

### 5.1.5. Mean fractional reduction of daily gross CH<sub>2</sub>O assimilation rate ( $A_{\max\text{red}}$ ) within the growing season

Figure 32-35 show that CH<sub>2</sub>O assimilation rates ( $A_{\max\text{red}}$ ) in wheat were reduced between 6-20 % in Bremen, and 2 and 20 % in Jerez, depending on water limited or fully irrigated conditions- in line with the reductions of biomass and green leaf area index. Likewise, in barley the reductions were much smaller.

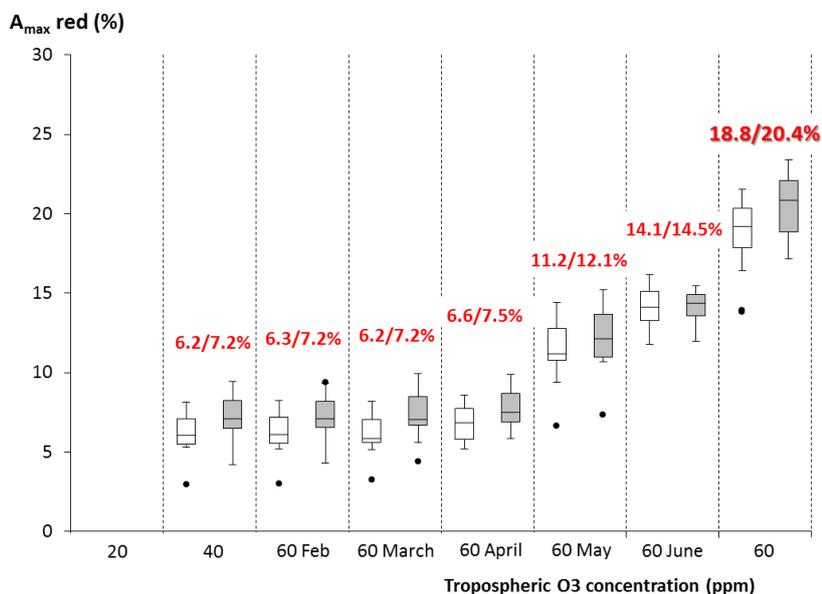


Figure 21. Boxplot of absolute mean values of  $A_{\max\text{red}}$  within the growing season, simulated for the pre-industrial, back ground and high ozone concentrations scenarios. Each box is derived from the 19 values simulated for wheat crop in Bremen, Germany. Open boxes refer to rainfed conditions, grey boxes to fully irrigated conditions.

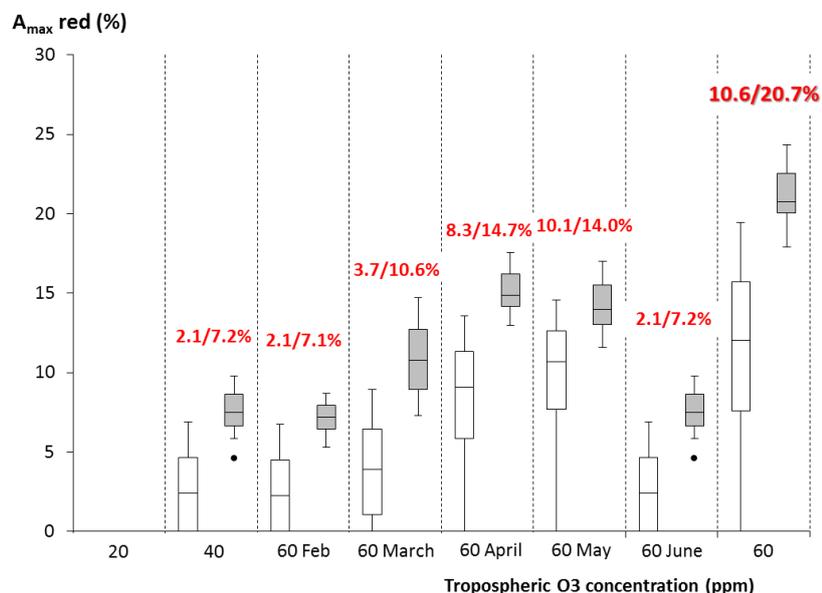


Figure 22. Boxplot of absolute mean values of  $A_{\max\text{red}}$  within the growing season, simulated for the pre-industrial, back ground and high ozone concentrations scenarios. Each box is derived from the 19 values simulated for wheat crop in Jerez de la Frontera, Spain. Open boxes refer to rainfed conditions, grey boxes to fully irrigated conditions.

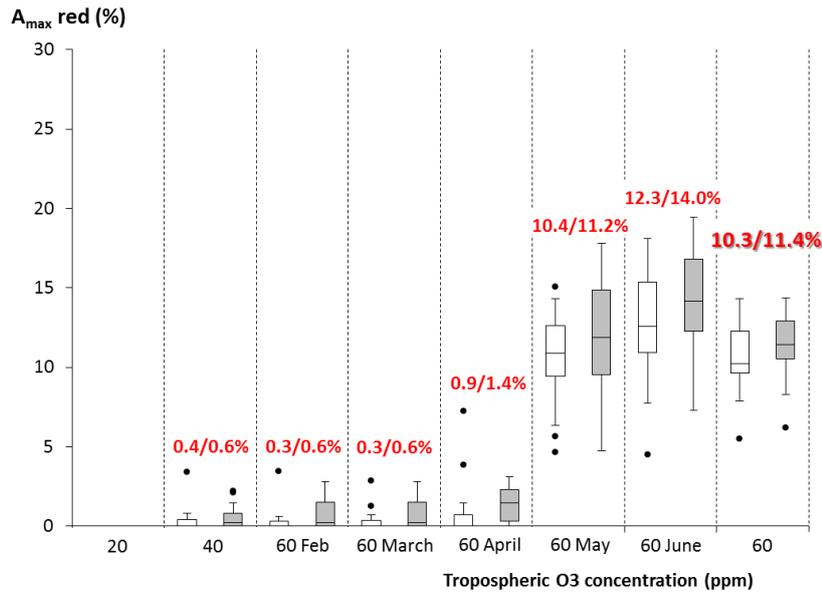


Figure 23. Boxplot of absolute mean values of  $A_{\max}$  red within the growing season, simulated for the pre-industrial, back ground and high Ozone concentrations scenarios. Each box is derived from the 19 values simulated for barley crop in Bremen, Germany. Open boxes refer to rainfed conditions, grey boxes to fully irrigated conditions.

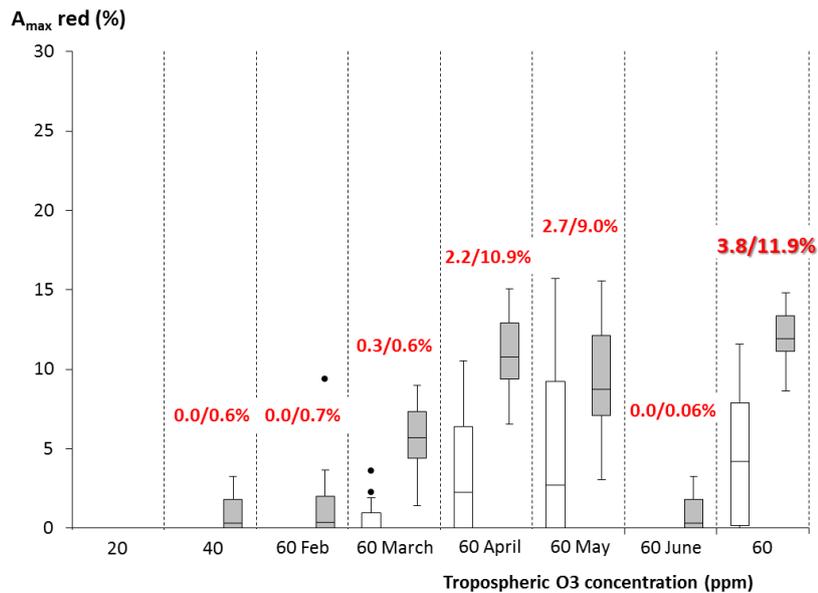


Figure 24. Boxplot of absolute mean values of  $A_{\max}$  red (%) within the growing season, simulated for the pre-industrial, back ground and high Ozone concentrations scenarios. Each box is derived from the 19 values simulated for barley crop in Jerez de la Frontera, Spain. Open boxes refer to rainfed conditions, grey boxes to fully irrigated conditions.

### 5.1.6. Cumulative ozone fluxes during the growing season ( $O_3$ cum fluxes)

Figure 36-39 show cumulative ozone fluxes during the growing season. As expected cumulative fluxes scale with the ozone concentrations, but are strongly down regulated under water limited conditions in Jerez. The anticipation of the growing cycle in Jerez compared to Bremen is clearly visible in the month of highest ozone flux.

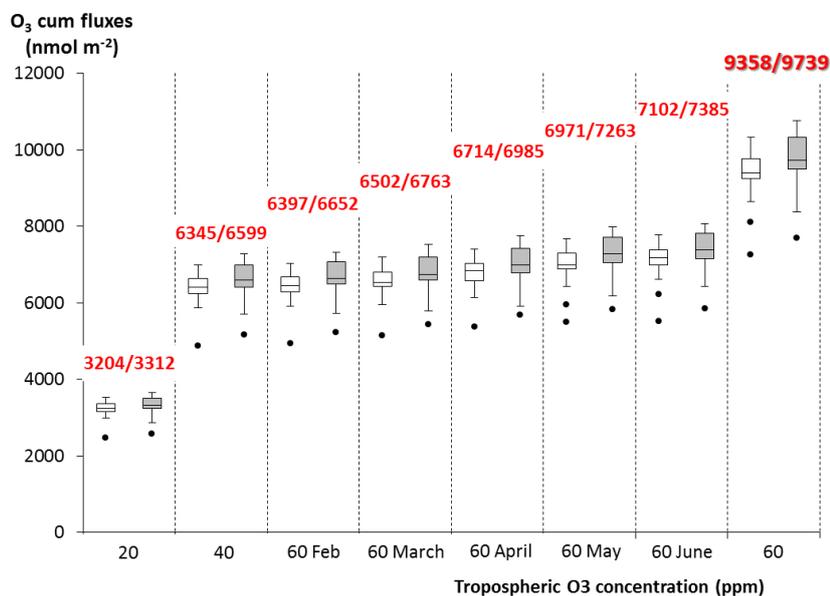


Figure 25. Boxplot of  $O_3$  cum fluxes ( $\text{nmol m}^{-2}$ ) simulated for the pre-industrial, back ground and high ozone concentrations scenarios. Each box is derived from the 19 values simulated for wheat crop in Bremen, Germany. Open boxes refer to rainfed conditions, grey boxes to fully irrigated conditions.

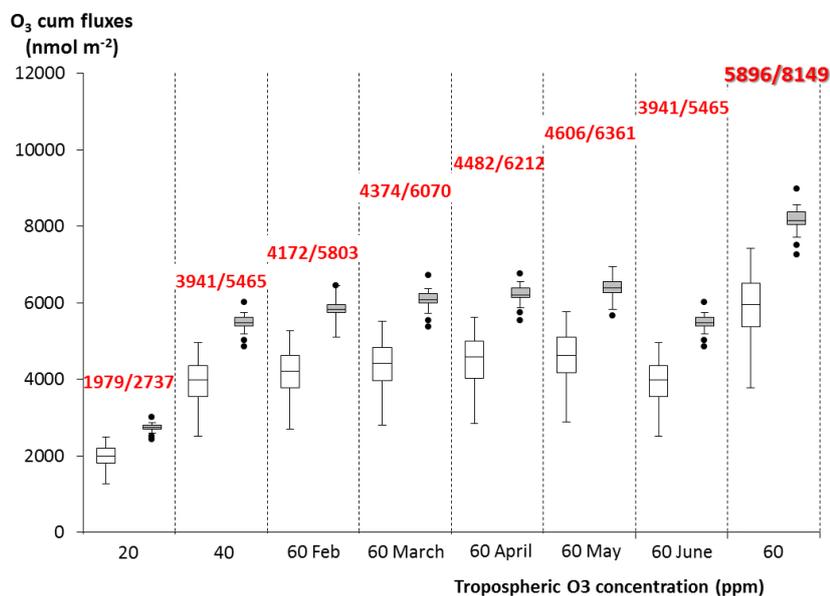


Figure 37. Boxplot of  $O_3$  cum fluxes ( $\text{nmol m}^{-2}$ ) simulated for the pre-industrial, back ground and high Ozone concentrations scenarios. Each box is derived from the 19 values simulated for wheat crop in Jerez de la Frontera, Spain. Open boxes refer to rainfed conditions, grey boxes to fully irrigated conditions.

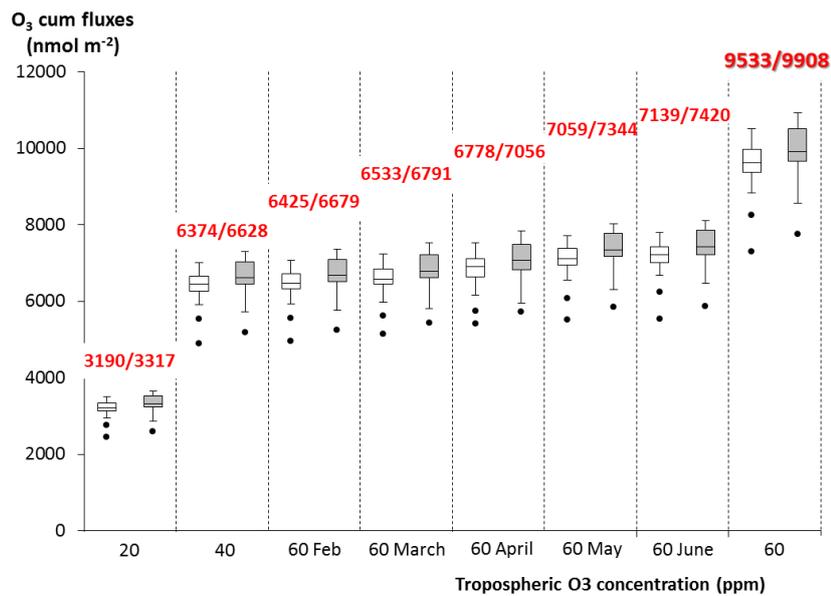


Figure 38. Boxplot of O<sub>3</sub> cum fluxes (nmol m<sup>-2</sup>) simulated for the pre-industrial, back ground and high Ozone concentrations scenarios. Each box is derived from the 19 values simulated for barley crop in Bremen, Germany. Open boxes refer to rainfed conditions, grey boxes to fully irrigated conditions.

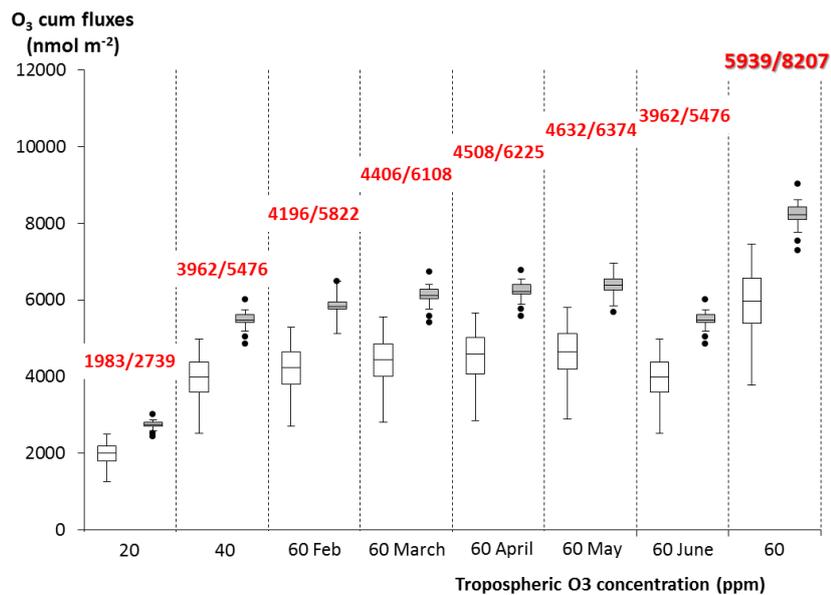


Figure 39. Boxplot of O<sub>3</sub> cum fluxes (nmol m<sup>-2</sup>) simulated for the pre-industrial, back ground and high Ozone concentrations scenarios. Each box is derived from the 19 values simulated for barley crop in Jerez de la Frontera, Spain. Open boxes refer to rainfed conditions, grey boxes to fully irrigated conditions.

A synthetic overview of the average variability in the 20-years simulated outputs as function of tropospheric O<sub>3</sub> concentration is given in Table 5, where all crop x variety x water management combinations are considered.

**Table 5. Comparison of model results concerning crop growth and damage due to ozone exposure under background and high O<sub>3</sub> tropospheric concentrations. The pairs of values refer to rainfed (left) and fully irrigated (right) conditions.**

Variable	Bremen		Jerez		unit
	Wheat	Barley	Wheat	Barley	
<b>Tropospheric [O<sub>3</sub>] 40 ppb</b>					
Yield*	-7.2;-9.3	-0.4;-0.3	-1.2;-6.4	-0.1;-0.1	%
AGB*	-5.0;-6.4	-0.2;-0.2	-0.7;-3.6	-0.1;-0.1	%
GLAI*	-2.7;-3.0	-0.4;-0.3	-1.4;-1.0	-0.2;-0.3	%
Days O <sub>3</sub> flux > [O <sub>3</sub> crit] <sup>°</sup>	64; 73	0.3; 1	14;-61	0; 1	d
Fractional Amax red <sup>°</sup>	-6.2;-7.2	-0.4;-0.6	-2.1;-7.2	-0.0;-0.6	%
Cumulative O <sub>3</sub> fluxes <sup>°</sup>	6345; 6599	6374; 6628	3941; 5465	3962; 5476	nmol m <sup>-2</sup>
<b>Tropospheric [O<sub>3</sub>] 60 ppb</b>					
Yield*	-29.4;-32.2	-11.7;-14.4	-11.8;-29.4	-1.3;-11.1	%
AGB*	-22.6;-25.0	-8.7;-10.8	-7.0;-19.3	-0.6;-6.0	%
GLAI*	-11.3;-12.8	-2.5;-3.1	-2.3;-5.4	-0.4;-0.8	%
Days O <sub>3</sub> flux > [O <sub>3</sub> crit] <sup>°</sup>	115; 118	74; 83	63;-97	20; 68	d
Fractional Amax red <sup>°</sup>	-8.8;-20.4	-10.3;-11.4	-10.6;-20.7	-3.8;-11.9	%
Cumulative O <sub>3</sub> fluxes <sup>°</sup>	9358; 9739	9533; 9908	5896; 8149	6939; 8207	nmol m <sup>-2</sup>

\* percentage difference compared to the pre-industrial scenario; ° absolute values

Based on the above analysis we can make the following general considerations regarding the behavior of the model developed:

1. in general crop damages due to O<sub>3</sub> exposure increase with O<sub>3</sub> concentration.
2. However, the effects of high O<sub>3</sub> concentrations are dependent crop, location, time of exposure simulated variable considered;
3. the highest impact is obtained when the month with high O<sub>3</sub> concentration coincides with the grain filling stage (June for Bremen, April for Jerez);
4. crop damages are more marked in Bremen than Jerez especially under rainfed condition.
5. irrigation practices exacerbate O<sub>3</sub> damages, especially in Jerez;
6. barley is less affected by O<sub>3</sub> impact according to the lower sensitivity of the crop.

## 6. Conclusions

The WOFOST crop model was extended with algorithms accounting for the effect of ozone on crop growth and yield. The extension encompassed the following elements: a) Effect of water stress on stomatal conductance, b) Ability of plants to recover from ozone damage c) Acceleration of leaf senescence due to O<sub>3</sub> exposure d) Reduction of green leaf area index due to foliar chlorosis or necrosis induced by O<sub>3</sub> e) Reduction of carboxylation rate of Rubisco, f) stomatal sluggishness (not implemented yet). Meteorological datasets with an hourly, and consistent daily resolution were provided for two locations in Germany (Bremen) and Spain (Jerez) encompassing different climatic conditions. To provide synthetic test conditions for the impacts of ozone, the plants were exposed to hypothetical O<sub>3</sub> levels of 20, 40, and 60 ppb during the entire crop growth cycle, and in separate sensitivity tests also for periods of one month to 60 ppb and to 40 ppb for the remainder of the growing season. Two crops were evaluated, wheat which is relatively sensitive to O<sub>3</sub>, and barley which is considered to be relatively O<sub>3</sub> insensitive. Two agro-management options were evaluated: fully irrigated (i.e. no water stress) and rain-fed. Irrespective of ozone, wheat and barley yields are lower by only 12 % in Bremen in the absence of irrigation, while reduced by 55 % in Jerez. Wheat yield losses up to 30 % are calculated for ozone concentrations of 60 ppb, and only half of these for barley. Yield losses are substantially smaller in Jerez for rainfed crops, when stomatal closure on the one hand is impeding crop growth and yields, but on the other reducing the impact of ozone. General findings regarding the model behaviour are: a) Crop damages due to O<sub>3</sub> exposure increase with O<sub>3</sub> concentration b) effects of high O<sub>3</sub> concentrations are very heterogeneous depending on month, site, crop and simulated variable considered c) the highest impact is obtained when the month with high O<sub>3</sub> concentration coincides with the maturity period (June for Bremen, April for Jerez) d) crop damage is more marked in Bremen than Jerez and irrigation practice exacerbates O<sub>3</sub> damages, especially in Jerez e) barley is less affected by O<sub>3</sub> impact according to the lower sensitivity of the crop. This behavior corresponds well with general findings in literature reviews on the subject, although only a qualitative comparison is possible on the basis of the *in silico* experiments conducted for this study. Further improvements are possible by:

- extending the model with algorithms to:
  - simulate stomatal sluggishness or disfunctioning, which might be induced at prolonged exposure to high ozone concentration, and
  - simulate the acute reduction of green leaf area index due to foliar chlorosis or necrosis induced by short-term very high doses of O<sub>3</sub>.
  - Account for the metabolic costs to plants to avoid (e.g. by producing antioxidants) or repair damage caused by ozone
- The model experiments were performed as sensitivity studies, to learn about model behaviour. Quantitative comparison of model results with real experimental data and with outcomes of more refined models that run with hourly time step.

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## 8. APPENDICES

### APPENDIX A. Patterns of meteorological variables in Jerez de la Frontera and Bremen

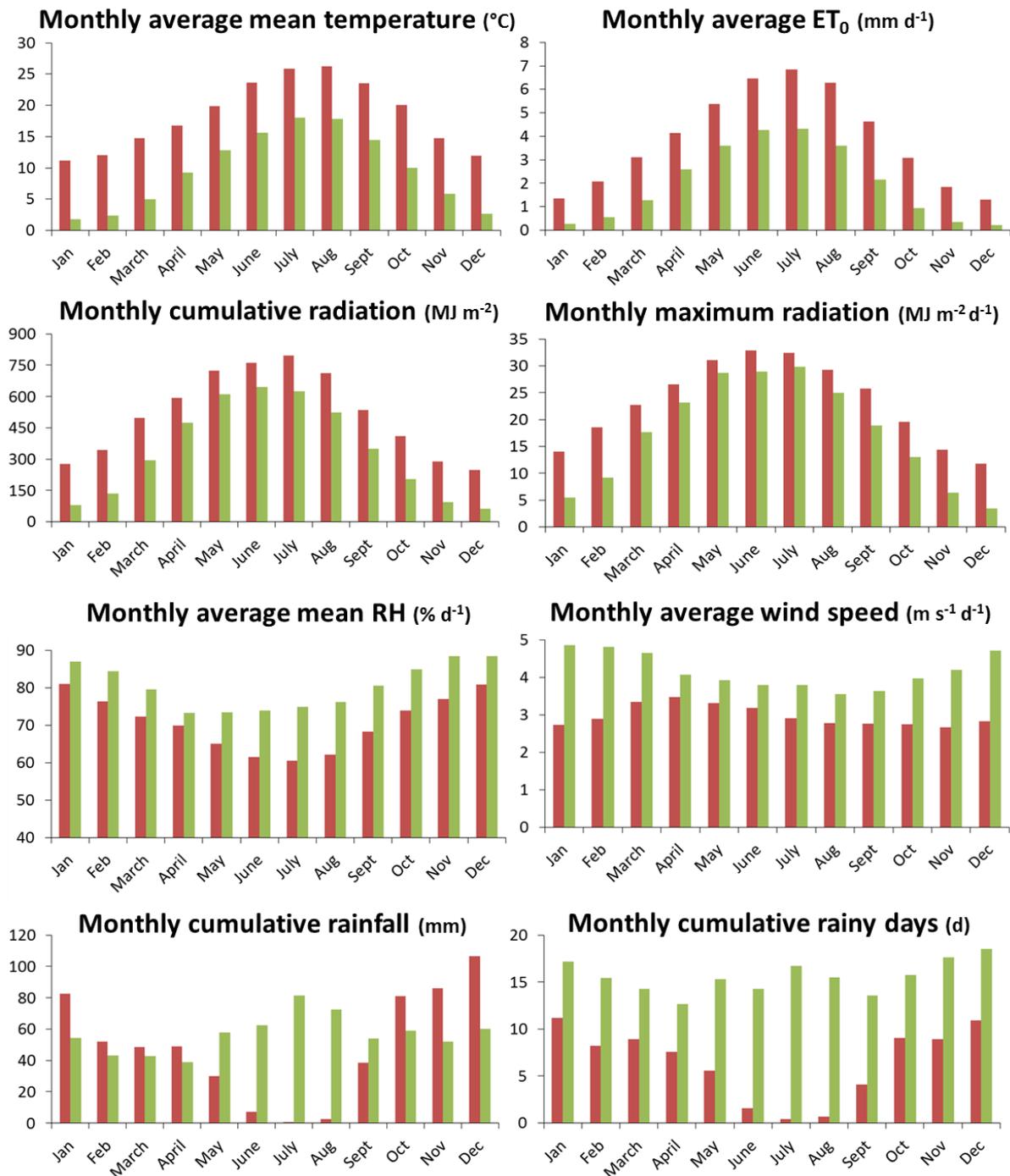


Figure A1 Monthly average values of the meteorological variables recorded by the stations located in Jerez de la Frontera (red bars) and Bremen (green bars) in the period 1996-2015

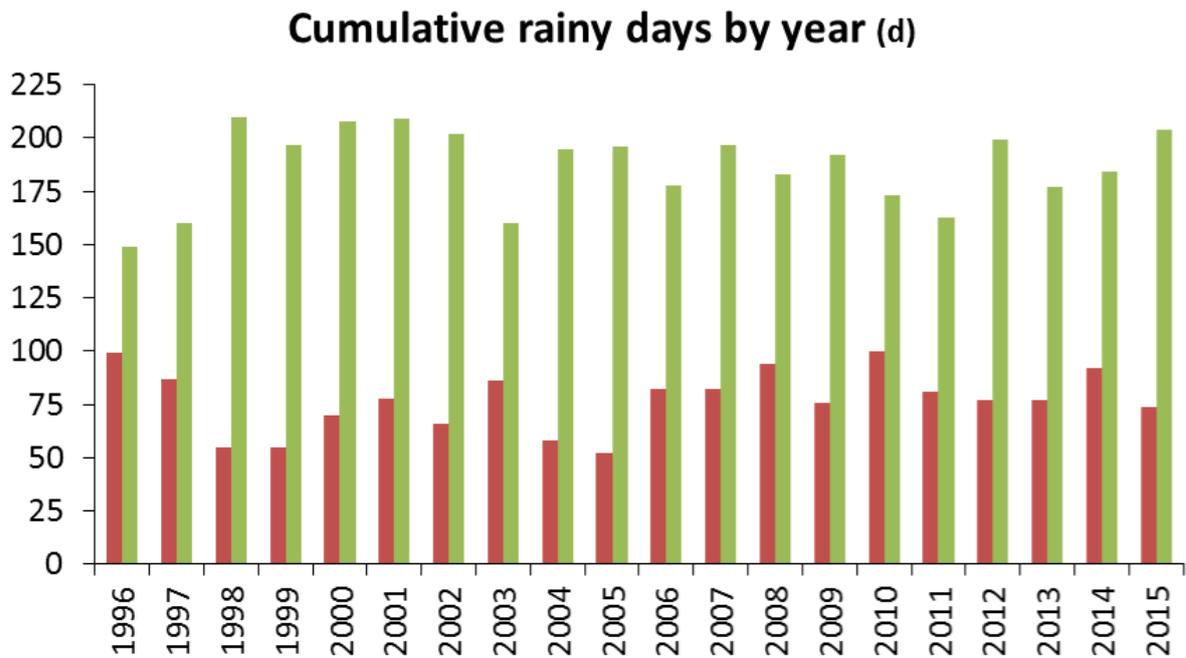
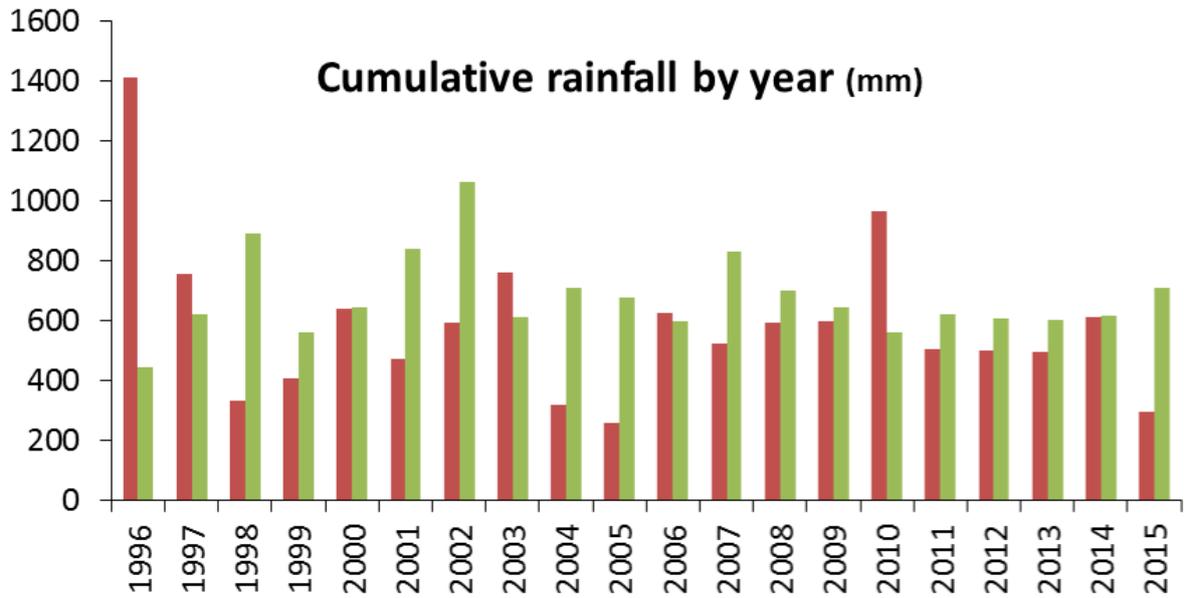


Figure A2. Seasonal values of cumulative rainfall and cumulative rainy days recorded by the stations located in Jerez de la Frontera (red histograms) and Bremen (green histograms) in the period 1996-2015.

## APPENDIX B. Short-term effect metacode

```
if (field.GreenLeafAreaIndex > 0)
{
    EstimateOfAssociatedClasses(ozone, impact, weather, field);

    ozone.O3FluxToStomata = Math.Max((ozone.O3FluxToStomata *
        ozone.WaterStressCoefficientStomata - PlantSpecificThreshold), 0);
    ozone.O3FluxToStomata *= hours_O3Uptake;

    _shorttermo3effect.Estimate(ozone, impact, weather, field);
}
foreach (GAIage GAI in field.LeafAreaIndexAge)
{
    double recoveryFromO3Damage_Fla = 1;
    if (GAI.PhysiologicAge_FYSDEL > 0)
    {
        recoveryFromO3Damage_Fla = 1 - GAI.PhysiologicAge_FYSDEL / GAI.SPAN;
    }

    double incompleteRecovery_R03s = GAI.ShortTermPhotosynthesis_O3 +
        (1 - GAI.ShortTermPhotosynthesis_O3) * recoveryFromO3Damage_Fla;

    double hourlyDecreaseAssimilation_F03h = 1;
    if (ozone.O3FluxToStomata > Gamma1/Gamma2 && ozone.O3FluxToStomata < (1+Gamma1)/Gamma2)
    {
        hourlyDecreaseAssimilation_F03h = Math.Min(1 + Gamma1 - Gamma2 * ozone.O3FluxToStomata, 1);
    }
    if (ozone.O3FluxToStomata >= (1+Gamma1)/Gamma2)
    {
        hourlyDecreaseAssimilation_F03h = 0;
    }

    GAI.ShortTermPhotosynthesis_O3 = hourlyDecreaseAssimilation_F03h * incompleteRecovery_R03s;

    for (int i = 0; i < hours_O3Uptake; i++)
    {
        GAI.ShortTermPhotosynthesis_O3 *= hourlyDecreaseAssimilation_F03h;
    }
}
double sumShortTermReduction = 0;
for (int i = 0; i < _runTimeData.CropMLDataType.States1_WOF0ST_WaterLim_short.LeafAreaIndexAge.Count; i++)
{
    _runTimeData.CropMLDataType.States1_WOF0ST_WaterLim_short.LeafAreaIndexAge[i].PhysiologicAge_FYSDEL =
    _runTimeData.AbioticDamageDataType.Field_short.LeafAreaIndexAge[i].PhysiologicAge_FYSDEL;
```

```

        _runTimeData.CropMLDataType.States1_WOFOST_WaterLim_short.LeafAreaIndexAge[i].AdjustedSPAN_03 =
_runTimeData.AbioticDamageDataType.Field_short.LeafAreaIndexAge[i].AdjustedSPAN_03;

_runTimeData.CropMLDataType.States1_WOFOST_WaterLim_short.LeafAreaIndexAge[i].ShortTermPhotosynthesis_03 =
_runTimeData.AbioticDamageDataType.Field_short.LeafAreaIndexAge[i].ShortTermPhotosynthesis_03;

        sumShortTermReduction +=
_runTimeData.CropMLDataType.States1_WOFOST_WaterLim_short.LeafAreaIndexAge[i].ShortTermPhotosynthesis_03;
    }

    double avgShortTermReduction = 1;

    if (_runTimeData.CropMLDataType.States1_WOFOST_WaterLim_short.LeafAreaIndexAge.Count != 0)
    {
        avgShortTermReduction = Math.Min(sumShortTermReduction /
_runTimeData.CropMLDataType.States1_WOFOST_WaterLim_short.LeafAreaIndexAge.Count, 1);
    }

_runTimeData.CropMLDataType.StatesExt_WOFOST_WaterLim_short.FractionalReductionOfPlantProduction_03 =
avgShortTermReduction;

```

## APPENDIX C. Long-term effect metacode

```
if (field.GreenLeafAreaIndex > 0)
{
    EstimateOfAssociatedClasses(ozone, impact, weather, field);

    ozone.O3FluxToStomata = Math.Max((ozone.O3FluxToStomata *
        ozone.WaterStressCoefficientStomata - PlantSpecificThreshold), 0);
    ozone.O3FluxToStomata *= hours_O3Uptake;

    _longtermO3effect.Estimate(ozone, impact, weather, field);
}

foreach (GAIage GAI in field.LeafAreaIndexAge)
{
    double ozoneFactor_f03l = Math.Max(1 - Gamma3 * GAI.CumulatedUptake_O3, 0);

    double AdjustedSPAN_yesterday = GAI.AdjustedSPAN_O3;
    GAI.AdjustedSPAN_O3 = GAI.SPAN * ozoneFactor_f03l;

    GAI.PhysiologicAge_FYSDEL += Math.Max((AdjustedSPAN_yesterday - GAI.AdjustedSPAN_O3), 0);

    double senescencePhase_Tlse = 0.33 * GAI.SPAN;
    double expansionPhase_Tlep = GAI.SPAN - senescencePhase_Tlse;

    GAI.LeafSenescenceFactor_O3 = 1;

    if (GAI.PhysiologicAge_FYSDEL > expansionPhase_Tlep)
    {
        GAI.LeafSenescenceFactor_O3 = Math.Max(1 - (GAI.PhysiologicAge_FYSDEL -
expansionPhase_Tlep) /
            (GAI.SPAN / ozoneFactor_f03l - expansionPhase_Tlep), 0);
    }

    GAI.CumulatedUptake_O3 += ozone.O3FluxToStomata / 1000;

double sumSPANReduction = 0;
    for (int i = 0; i <
_runTimeData.CropMLDataType.States1_WOF0ST_WaterLim_long.LeafAreaIndexAge.Count; i++)
    {
        _runTimeData.CropMLDataType.States1_WOF0ST_WaterLim_long.LeafAreaIndexAge[i].PhysiologicAge_FYSDEL =
_runTimeData.AbioticDamageDataType.Field_long.LeafAreaIndexAge[i].PhysiologicAge_FYSDEL;

        _runTimeData.CropMLDataType.States1_WOF0ST_WaterLim_long.LeafAreaIndexAge[i].CumulatedUptake_O3 =
_runTimeData.AbioticDamageDataType.Field_long.LeafAreaIndexAge[i].CumulatedUptake_O3;

        _runTimeData.CropMLDataType.States1_WOF0ST_WaterLim_long.LeafAreaIndexAge[i].AdjustedSPAN_O3 =
_runTimeData.AbioticDamageDataType.Field_long.LeafAreaIndexAge[i].AdjustedSPAN_O3;

        _runTimeData.CropMLDataType.States1_WOF0ST_WaterLim_long.LeafAreaIndexAge[i].LeafSenescenceFactor_O3 =
_runTimeData.AbioticDamageDataType.Field_long.LeafAreaIndexAge[i].LeafSenescenceFactor_O3;
```

```
        sumSPANReduction +=
_runTimeData.CropMLDataType.States1_WOFOST_WaterLim_long.LeafAreaIndexAge[i].AdjustedSPAN_03 /
Wofost.LifeSpanOfLeavesGrowingAt35Celsius_SPAN;
    }

    double avgSPANReduction = 1;

    if (_runTimeData.CropMLDataType.States1_WOFOST_WaterLim_long.LeafAreaIndexAge.Count != 0)
    {
        avgSPANReduction = Math.Min(sumSPANReduction /
_runTimeData.CropMLDataType.States1_WOFOST_WaterLim_long.LeafAreaIndexAge.Count, 1);
    }

    _runTimeData.CropMLDataType.StatesExt_WOFOST_WaterLim_long.FractionalReductionOfSPAN_03 =
avgSPANReduction;
}
```

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