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Evaluation of the LPJ-GUESS crop model under ambient and elevated CO_2 concentrations.

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Abstract

In the future atmospheric CO_2 concentrations might exceed 550 ppm according to the RCP8.5 scenario by mid-century from our current 410 ppm, while our world population is projected to surpass the 9.7 billion threshold within the same time span. This challenge leads to the raising of questions addressing future food security.

Elevated CO_2 has been shown to not only increase photosynthetic rates in plants, but also to reduce stomatal conductance where both processes generate increases in biomass and yield. In this thesis, the performance of the LPJ-GUESS crop model in simulating observed wheat yields under both ambient and elevated CO_2 concentrations has been evaluated. Observational data has been obtained from three free-air carbon dioxide enrichment (FACE) facilities, located in Germany, the United States of America and Australia. Model benchmarking revealed issues regarding yield underestimation which were consistent for both ambient and elevated CO_2 model runs. Nonetheless, the model managed to capture the CO_2 response reasonably well. The simulated yields for the German site provided the best agreement between modelled and observed data, with a CO_2 response of 12% compared to the 15% in field, when CO_2 concentrations were increased by 180 ppm. Conversely, the American site led to the lowest agreement, due to strongly underestimated yields and a CO_2 response of 33% (instead of 15%) that led to an average modelled yield increase of 2 t/ha once exposed to elevated CO_2.

Furthermore, modelled leaf area index (LAI) development is consistently delayed by about 1.5 months for all locations. Water stress has been found to primarily affect wheat towards the end of the growing season in Australia, while some influence could be observed in the US as well. After exposure to elevated CO_2, improvements in water stress levels could be noted. A comparison between field measurements of gross primary productivity (GPP), revealed that GPP is underestimated by 37%, while simulated net primary production (NPP) fluxes are overestimated by 25% in LPJ-GUESS. An offset of NPP in the beginning of the growing season leads to most of the NPP and biomass accumulating in a shorter time window towards the end of the growing period.

To be able to utilise this model for future crop grain estimates, issue regarding the underestimating yields and delayed LAI need to be solved first. Otherwise, it will become challenging to successfully project yields for future climate scenarios, where elevated CO_2, increased temperature, and drought might interact simultaneously at the end of the growing period. As this is the period, where most of the biomass is accumulating, even lower yield estimates can be expected. In the future advances and improvements in crop growth models will become more important, which depend on availably of field data of high quality for purposes such as model validation and calibration, stressing the responsibility of experimentalists to include as many relevant measurements as possible.

Table of Contents

1 Introduction

Future climate estimations suggest that carbon dioxide (CO_2) concentrations will keep rising from their current level of 410 ppm to 550 pm by mid-century under the RPC 8.5 scenario (Stocker, 2014). To add on climate change does not only alter atmospheric CO_2 concentrations but includes rising temperatures and increases in extreme weather events. With droughts and heatwaves occurring more frequently, many cropping regions of the world will be negatively affected (Field et al., 2014). This challenge is only amplified by projections from the United Nations revealing that the world's population might bypass the 9.7 billion threshold within the same time frame (UN, 2019). Further strengthening concerns about food security, as a stronger emphasis will have to be set on enhanced crop production to meet the nutritional requirements of the growing population.

When addressing the future nutritional status of our society, an important crop to investigate is wheat, which is the dominating crop from a land usage perspective, occupying a cultivated area of 219 million hectares and accounting for a worldwide production of 761 million tonnes in 2020 (FAO, 2020). Therefore, it is crucial to gain knowledge about the response of these plants to enhanced CO_2 concentrations and to gather an understanding of their adaptational ability, in order to obtain insight on how the multiple stressors of climate change might influence ecosystems as a whole. Moreover, humankind relies on services provided by these environments for purposes including nutrition, drinking water, fuel, and fresh air. Additional knowledge about how plants might respond to the predicted increase in CO_2 concentrations has been acquired with the help of diverse carbon enrichment studies organised throughout the last 30 years (Leakey et al., 2009).

With increasing CO_2 concentrations in the atmosphere, photosynthesis rates of plants are rising, meaning that crops will produce more biomass and higher yields. However, to quantify these changes and responses to elevated $CO_{2,}$ it is necessary to conduct studies and collect data, which is where free-air carbon dioxide enrichment experiments (FACE) come into play. FACE is a unique experimental setup, which exposes plants to elevated CO_2 in a natural environment with the help of horizontal pipes, emitting CO2 into the plots. (Ainsworth & Long, 2005).

It is unattainable to administer FACE experiments for each unique blend of climate, soil properties and crop species, to project what could happen in the future on a local or global scale. For this reason, advances in crop growth models are becoming crucial to being able to successfully replicate the impact of enhanced CO_2 levels and additional climatic changes on crop development and yield (Kimball et al., 2002). Due to the models' need for validation, data from FACE experiments is required, to investigate whether simulated yields are within reason (Kimball et al., 2002).

One model that could shed light upon this rising global concern is LPJ-GUESS, a dynamic global vegetation model, whose use has been widespread in the scientific community with over 450 peer-reviewed publications up to date (Lund-University, 2022). It is constantly being developed in order to better represent ecosystem processes. Inclusions worth mentioning are for example the possibility to simulate cropland in the managed land version incorporated by Lindeskog et al. (2013) and the incorporation of the nitrogen cycle by Olin et al. (2015). Throughout the years, different model versions of LPJ-GUESS have been evaluated in studies addressing the impact of elevated CO_2 on plants (Olin et al., 2015; Smith et al., 2014), seasonality of vegetation (Lindeskog et al., 2013) and ecosystem carbon response to climate change projections (Ahlström et al., 2012).

1.1 Aim and Objectives

The aim of this thesis is to evaluate how well the LPJ-GUESS crop model can simulate observed yields under both ambient and elevated CO_2 concentrations. Furthermore, the strength of the modelled CO_2 response will be placed into context by comparing obtained results to observational data. After the initial benchmark process, daily outputs will be investigated in order to find shortcomings in the model and suggest potential development opportunities to be facilitate future yield simulations and subsequent estimations.

1.2 Research questions

1. How well can LPJ-GUESS simulate observed yields under ambient and elevated CO_2 concentrations? How strong is the modelled CO_2 response?
2. What are the reasons for the differences between model and observations? Where could improvements be made?

2 Background

Factors later examined that might have an impact on phenological development and influence grain production will be presented in this section. Firstly, the introduction of concepts such as the carbon fertilisation effect will grant some insight into how elevated atmospheric CO_2 concentrations lead to higher productivity. Subsequently, the benefits of free-air CO_2 enrichment experiments (FACE) to conventional enclosure studies will be elaborated.

2.1 Carbon fertilisation effect

In the past multiple studies have been executed that aimed to model the consequences of a changing climate with increasing CO_2 concentrations on global and local food security (McGrath & Lobell, 2013). Throughout these studies, one of the major findings has been that food production is not only influenced by the mean global effect of climate change but also the local variability and specific impacts of climate change there. This local effect plays a crucial role for competition in global trade (Hertel et al., 2010; Rosenzweig & Parry, 1994). It has been found that the carbon fertilisation effect (CFE) relies on crop type and soil moisture availability. Given the spatial variability of these two parameters, CFE should also possess this spatial characteristic (McGrath & Lobell, 2013).

Most plants, when performing photosynthesis follow the C_3 pathway, which has acquired its name from the first transformation of CO_2 which leads to the formation of a new molecule containing 3 carbon atoms (Smith et al., 2001). The enzyme Rubisco acts as catalyst and is therefore responsible for the initial chemical reactions to occur, where CO_2 gets transformed into carbohydrates. However, if oxygen in molecular form is available, Rubisco can start a process called photorespiration. During this reaction, energy gets consumed instead of produced, while CO_2 simultaneously gets released (Smith et al., 2001). Due to the fact that Rubisco, has not reached saturation under current CO_2 concentrations yet, elevated CO_2

promotes the assimilation of carbon (Kimball et al., 2002). Furthermore, enhanced CO_2 prevents Rubisco from reacting with O_2, lowering the amount of CO_2 released during photorespiration (McGrath & Lobell, 2013). Another factor to consider is that under elevated CO_2 concentrations of around 567 ppm leads to a decrease of stomatal conductance of 22% in C_3 plants (Ainsworth, 2007), which lowers water lost on the canopy level (Leakey et al., 2009) and might promote crop productivity under water deficient conditions (Fitzgerald et al., 2016; Kimball et al., 2002). Thus, elevated CO_2 concentrations would lead to a reduction of photorespiration, favouring the productivity of C_3 plants (Smith 2001).

Generally, C_3 species respond with yield increases under elevated CO_2 levels due to multiple factors, including lower photorespiration, improved water use efficiency and enhanced rates of binding atmospheric CO_2 to sugars (carboxylation) (Ainsworth & Long, 2005). In addition, C_3 crops have been observed to attain higher CO_2 responses in water limiting environments as opposed to irrigated systems or other non-water limiting areas (Kimball et al., 2002).

It has been noted by McGrath and Lobell (2013), that dynamic vegetation models utilised for future crop estimations, should improve yield simulations on a field scale. Despite this need for improvement studies disagree on the predicted extent these local responses should have and the amount regarding how much the regional carbon fertilization effect (CFE) might fluctuate (McGrath & Lobell, 2013). Moreover, these discrepancies between CFE prevents the forming of concise answers when it comes to identifying the cause behind local yield changes, which might be due to the impact of climate change or due to the impact of elevated CO_2 concentrations as a single factor. In fact, differences in yield due to climatic influence are more than 9 times as variable throughout regions than yield increases due to the impact of enhanced CO_2 concentrations (Fischer, 2009) while in a study conducted by Müller et al. (2010) yield changes possessed more variability as a consequence of changes in CO_2.

Another reason behind regional fluctuations of CFE might be caused by the amount of nitrogen present. Regions that are not nitrogen limited, have been shown to have a higher CFE than locations where nitrogen availability is insufficient (Ainsworth & Long, 2005). This difference occurs due the fact that when nitrogen does not act as a limitation for crop development, the observed CFE can be understood as the upper limit of the response to elevated CO_2 (McGrath & Lobell, 2013).

In order to close the gap and obtain understanding on the local CFE, additional studies should be conducted, which focus on the interplay between elevated CO_2 and drought stress, especially to analyse the relationship between temperature and CO_2 (McGrath & Lobell, 2013).

2.2 Free-Air Carbon Dioxide Enrichment Experiments (FACE)

Since atmospheric concentrations of CO_2 have been increasing, questions regarding potential implications for plants and the entire ecosystem once exposed to this have arisen. Subsequently initiating research with the goal to unpack and obtain knowledge about their potential response (Ainsworth & Long, 2005).

Firstly, the main plant processes impacted by elevated CO_2 are well established and affected are parameters such as deceased transpiration and stomatal conductance, enhanced photosynthetic rates, as well as increased water and light-use efficiency (Drake et al., 1997).

However, the majority of these results were drawn from studies conducted on plants in controlled systems such as open-top chambers, where in and outflow of air is restricted due to physical boundaries, giving rise to substantial limitations. Examples of such limitations in enclosure studies are an enhanced decrease in sensitivity for photosynthetic processes and productivity, which occurs due to the plant's acclimation to elevated CO_2 concentrations (Morgan et al., 2001). Hence, photosynthetic acclimation decreased the favoured position of plants grown in elevated CO_2 chambers to such a degree that photosynthesis rates were almost identical to plants grown under ambient levels (Morgan et al., 2001). Another issue of the enclosure setups to consider is that the manually modified environment might generate a "chamber effect" possibility even surpassing the effect of increased CO_2. Having size constraints in place, might confine root space; thus restraining the CO_2 response (ARP, 1991).

Therefore, free-air CO_2 enrichment (FACE) facilities were installed to tackle these limitations originated from enclosure systems by exposing plants to elevated CO_2 in a more natural setting under open air, as it does not rely on constraining setups (Ainsworth & Long, 2005). Instead CO_2 enrichment occurs via multiple horizontal and vertical pipes that either blow the required amount of CO_2 concentrated air into the system or release clean CO_2 gas at the edge of the experimental plots (Ainsworth & Long, 2005). In the FACE systems, turbulence in the air is responsible for spreading the CO_2 throughout the plots with the help of diffusion processes. Throughout the last decades numerous FACE studies have been carried out subjecting plants to CO_2 concentrations between 475-600 ppm. Included in these experiments are treatments on different species belonging to diverse plant functional group, various fertilizer applications and other types of stress exposure (Ainsworth & Long, 2005).

2.3 Factors influencing wheat development

Wheat is a globally widespread crop that can grow under various climatic conditions, including temperate, warm, cold and locations with different levels of water availability. Since wheat utilises the C3 photosynthetic pathway, it prefers colder climate regimes (Acevedo et al., 2002). Due to its presence all over the world, wheat poses as one of the most studied crops regarding FACE studies, which allowed for the assessment of different stress treatments and provided data to be used in model validation studies.

Wheat development starts with germination, which can only occur if a minimum of 35-45% of the grain's weight is occupied by water (Evans et al., 1975). Furthermore, temperatures in the range of 4° to 37°C allow germination to take place, while the optimum range lies between 12° and 25°C. The initial growth starts with the seminal roots, accompanied afterwards by the development of coleoptile, which is responsible for sheltering the first leaf from emergence. The main shoot leaves' point of divergence acts as place of origin for crop tillers to emerge and the number of tillers present depends on cultivar, where winter species tend to have a larger amount (Acevedo et al., 2002). Afterwards tillers give rise to wheat spikes, but most of them do not participate in spike production and break off prior to anthesis (Gallagher & Biscoe, 1978). Typically, one to one-half productive tillers reach the anthesis stage, which can vary due to climatic and planting environments. Then the vegetative stage (GS1) starts, which takes places for 60 to 150 days, governed by cultivar type and sowing date (Acevedo et al., 2002). This stage is controlled by phyllochron (leaf appearance rate) and timing of the double ridge (individual flower development), initiated by processes such as vernalization and photoperiod. Where leaf appearance rate is described as the time interval between two consecutive leaves in the identical stem obtaining a comparable development stage (Acevedo et al., 2002).

Generally, crop development can be characterised by growing degree-days (GDD), where a base temperature between 0° and 4°C is used for physiological processes. Thus,

$$(1)\ GDD = [(T_{max} + T_{min})/2] - T_b$$

where T_{max} and T_{min} denotes the daily maximum and minimum temperature and T_b the base temperature (Cao & Moss, 1989). The GDD change depending on growing stage and therefore can be utilised as an estimate of the timing of a certain development stage of a specific location.

Winter wheat only start to flower after being exposed to a period of colder temperatures, this phenomenon is called vernalization. Typically, temperature in the range of 0° to 12°C are needed for vernalization to take place. On the other hand, spring wheat has shown to have a considerably small reaction or even no reaction to vernalization and has low tolerance for frost (Acevedo et al., 2002).

Once vernalization takes place, some species need a particular amount of day-length to induce flowering, due to the being responsive to photoperiod (Acevedo et al., 2002). However, the level of sensitivity varies across cultivar and most wheat types do not rely on a specific day-length but tend to initiate flowering at faster rates once the days get longer (Evans et al., 1975). The photoperiod concludes the vegetative stage, afterwards the double ridge starts, which is defined as the beginning of the reproduction phase. In this stage florets in the spikelets develop, which will be later fertilized. The next stage initiates the formation of the terminal spikelet, followed by the stem elongation and finally the spike starts growing (Acevedo et al., 2002). Once Anthesis starts, the wheat spike consists of one spikelet, which has three to six florets that could be fertilised (Kirby & Appleyard, 1981). When fertilization is finished, a lag phase which is taking up 20-30% of the total grain filling phase occurs, where cellular division happens in order to give rise to cell growth and starch accumulation, occupying the remaining part of the grain filling period (Acevedo et al., 2002).

Water stress is a frequent stressor in the natural environment, it arises when crops consume less water than the atmosphere requires from them in evaporation. There are two essential mechanisms at play; firstly, the crop's water consumption governed by physical characterises of the soil and root traits and the crop's evapotranspiration, which relies on atmospheric conditions such as vapour pressure deficit and net radiation, but also crop properties, which include ground coverage and stomatal conductance. To add on, crop transpiration is found to have a positive linear relationship to yield, thus water stress leads ultimately to lower production (Acevedo et al., 2002).

2.4 LPJ-GUESS description

In order to simulate crop yield responses under elevated CO_2 levels the process-based dynamic vegetation model LPJ-GUESS v4.1 has been utilised, which is suitable for regional and global ecosystem modelling purposes (Smith et al., 2014). In addition, the model is not only capable of describing dynamic vegetation and soil processes, but also their responses in exchange following changes in management practise or environmental modifications. These changes included are for example in CO_2 concentration levels, climate, soil characteristics, deposition and fertilization of nitrogen. Some processes determining the simulated vegetation stand are calculated daily, such as photosynthesis, respiration, and stomatal conductance, while others such as net primary production (NPP) are estimated yearly. Different inputs are necessary to be able run the model, which include climate data in the form of temperature, precipitation and solar radiation, soil characteristics and CO_2 concentrations (Smith et al., 2014).

It is possible to simulate three distinctive land-use categories, such as natural vegetation, pastures, and croplands. With the help of 12 plant functional types (PFT) natural vegetation can be described, and vegetation generated in the model follows processes from establishment, through growth towards the end of their life cycle. The competition of different C_3 and C_4 grasses is used to model pastures, where grazing is simulated by harvesting half of the aboveground biomass yearly (Lindeskog et al., 2013). For the simulation of croplands, different management practises are available to be incorporated, such as supplementary irrigation, addition of nitrogen fertilizer, tillage, grass cover amid two growing periods, and crop residue management (Olin et al., 2015; Pugh et al., 2015). This version of LPJ-GUESS proceeds from the concept and computations established in the previous version, along with carbon cycle and nitrogen cycle calculations (Olin et al., 2015; Smith et al., 2014). The nitrogen cycle has been incorporated to be able to simulate processes such as nitrogen stress, which was not the case in the C-only version and led to highly overestimated yields (Rosenzweig et al., 2014). Thus, it is possible to not only calculate where crops allocate their carbon (roots, leaves, harvestable parts) but also nitrogen on a daily basis.

The diversity of crops species is accounted for in LPJ-GUESS within the managed land version (Lindeskog et al., 2013) by distinguish between different crop plant functional type (CFTs). Crops that are placed in the same CFT share crucial characteristics, such as photosynthetic pathway (C_3 or C_4), preferred climatic regime and their carbon allocation pattern. Wheat belongs into the same CFTs, which represents temperate C_3 crops, including winter cereals, barley, rye and oats. These are further separated based on whether sowing takes place in spring (TeSW) or autumn (TeWW). If sowing dates are not set manually, the model can determine these depending on the grid cell's dominant climate conditions. Harvest on the other hand occurs once crop potential heat unit requirements (PHU) are satisfied (Lindeskog et al., 2013). The amount of PHU necessary to reach crop maturity, is computed dynamically with the help of a decadal running mean obtained from summarized heat units (degree days over base temperature, T_b) gathered within the interval between sowing and harvest (190 to 245 days) (Lindeskog et al., 2013).

Instead of modelling crop phenological development depending on weather, development stages are utilised in LPJ-GUESS, allowing the growing period to be more precisely distributed to their corresponding crop development stage (Wang & Engel, 1998). The development stage (DS, (Wang & Engel, 1998)) is expressed through a value between 0 to 2, with the interval between 0 and 1 representing the vegetative stage, at $D=1$ anthesis takes place and $DS>1$ characterises the grain filling stage. A benefit of the DS implementation is that times during crop development that are specifically vulnerable to stressor, such as nitrogen limitation or heat strain are able to be depicted in more detail. Moreover, the crop's development stage plays an essential role for carbon allocation, which depends on incoming radiation (day length) and temperature (Olin et al., 2015).

When allocating the amount of daily carbon to different plant parts during the crop growing period, LPJ-GUESS depends on the allocation computations established by Vries (1989). Instead of utilising a function that is set to reach a fixed value at the end of the growing phase, carbon allocation is linked to daily NPP and DS. In the beginning of the vegetative stage, corresponding to $DS<0.7$ (for winter wheat), the majority of carbon gets allocated to the leaf and roots, enabling their growth by absorbing large quantities of nutrients, water and incoming radiation to photosynthesise. While in the second part carbon primarily assimilates in the stem. Once anthesis (DS>1) took place, the grain filling stage gets initiated, where the storage organs are the dominant receiver of carbon, at the same time crops tend to transport nutrients from their vegetative parts to the grain (Bertheloot et al., 2008). However, if the plant is exposed stressors, such as water deficit or nutrient limitation during their vegetative stage, more carbon gets allocated to the roots to make up for the deficits (Van Keulen et al., 1989). Therefore, roots need to be simulated independently from other plant parts.

3 Model set-up

Observational data for crop yield responses under elevated CO_2 were collected, to be able to evaluate how well LPJ-GUESS can simulate these yield increases. Different locations have been chosen where FACE experiments have been conducted, which include experimental sites in the United States of America, Australia, and Germany. These areas were investigated due to their spatial and climatic variability, as well as the fact that observational data was collected within the time window covered by the climatic data set (1901-2015).

During the enrichment phase CO_2 concentrations in the free air were increased to 550 ppm, while yields under ambient levels were also investigated for comparison purposes. Furthermore, management practices differed between the locations and were accounted for in the model runs, these treatments include but are not limited to applications of fertilisers, sowing times, and supplementary irrigation (Fig. 1). As none of these sites gathered data about gross primary productivity (GPP), nor net primary productivity (NPP) an additional simulation for a cropping system in western Germany was run to analyse the modelled GPP and NPP against field data.

Table 1. *Overview of the all the experiments run in LPJ-GUESS.*

Location	Growing period	Ambient/Elevated CO2	Nitrogen treatment	Irrigation	Sowing time
Braunschweig, GER	2001/2, 2004/5	both	high/low	yes	one
Maricopa, USA	1995/6, 1996/7	both	high/low	yes	one
Walpeup, AUS	2008, 2009	both	none	no	two
Selhausen, GER	2007/8, 2008/9	ambient	medium	no	one

As climate data is required for the model to run, the gridded CRU TS 4.0 (1901-2015) global climate data set (Harris & Jonas, 2017) was used for all locations. The soil data set WISE 3.0 (Batjes, 2005) was utilised, which provides fraction of sand, silt and clay present in the soil on a 0.5 by 0.5 degree grid. For input of global atmospheric nitrogen deposition, the dataset (Lamarque et al., 2010) obtained from the Atmospheric Chemistry and Climate Model Intercomparison Project (ACCMIP) was used, which supplied monthly deposition averages changing every ten years.

For the ambient CO_2 simulations, historical CO_2 concentration levels from 1901-2018 were applied, while for the elevated CO_2 simulations the historical data was manipulated reaching levels of 550 ppm for the time duration where the individual FACE experiments took place. In this version of the model the crops are run in the spin-up phase, which takes around 500 years and utilises observation-based, interpolated climate data (1901-2015) and CO_2 as forcings.

In this study two temperate C_3 crops were investigated, namely winter wheat (TeWW) and spring wheat (TeSW), where the major distinction between the types is found in sowing and harvest dates, as well as timing of fertilizer application. Furthermore, the parameters relevant for plant carbon allocation for these two CFTs were calibrated through a globally calibrated wheat version (Carmargo et al., in prep.). Crop cover then was set to represent each CFTs present in the individual patches as a fraction of 1. Since the number of patches was not adjusted, the default set up for one patch of 0.1 ha size was used.

3.1 Site description and setup

The four main locations for the LPJ-GUESS stimulations will be introduced, as well as knowledge regarding how diverse treatments applied at the FACE facilities and eddy covariance study site were modelled.

3.1.1 Braunschweig, Germany

The German FACE experimental setup consists of an agricultural field of 20 ha in size, located close to Braunschweig at 52.8°N, 10.8°E. During two growing season 2001/2 and 2004/5, the enrichment experiment took place on the cultivar Batis, a typical winter wheat species grown in the county. To diminish the potential influence of drought stress and its interactions with enhanced CO_2 treatment, the plots were irrigated. (Weigel & Manderscheid, 2012).

Then in LPJ-GUESS four different experimental treatments were simulated, high and low nitrogen fertilizer input under ambient and elevated CO_2 concentrations respectively. Given the fact that only information about the total amount of fertilizer is provided and details regarding timing and individual application are missing, these variables had to be manually adjusted according to the findings of a study conducted by Olin et al. (2015). Thus, fractions of the total fertilizer addition were set to take place with 19% applied halfway through anthesis and 73% close to anthesis, while the remaining amount to assumed to be added during sowing. The table below are the crop management details summarized (Table 2).

Table 2. *Management practises for the FACE experiment in Braunschweig, Germany.*

Management	Units	2001/2002 Wheat	2004/2005 Wheat
Sowing	Date	06.11.01	26.10.04
N-fert. (H/L)	kg/ha	251/114	168/84
Final Harvest	Date	31.07.02	27.07.05
CO2 (ambient/elevated)	ppm	377/550	378/550

3.1.2 Maricopa, USA

The FACE facility in Maricopa, Arizona is located at 33.1°N, 112.0°W. The winter wheat cultivar Yecora Rojo, was grown between the years 1995 to 1997 under two different nitrogen fertiliser regimes (high and low), while both treatments also included the application of supplementary irrigation (Kimball et al., 2016).

Once again four experimental trails were simulated (Table 3). As no explicit harvest date was provided, the model was run without this forcing and the harvest date modelled was reached once heat sum requirements were met. Since the provided dataset included information with the concrete timing and amount of fertiliser applied, these parameters were set accordingly for the different trials. Thus, the calculated percentages of the total applied fertiliser amount were 21% and 14% received halfway to anthesis and 78% and 85% close to anthesis, for the low and high nitrogen treatment respectively (Kimball et al., 2016).

Table 3. *Management practises for the FACE experiment in Maricopa, USA.*

Management	Units	1995/1996 Wheat	1996/1997 Wheat
Sowing	Date	15.12.95	15.12.96
N-fert. (H/L)	kg/ha	383/100	393/53
Final Harvest	Date	/	/
CO2 (ambient/elevated)	ppm	370/550	370/550

3.1.3 Walpeup, Australia

Walpeup, one of the two study sites of the AGFACE project is placed in the main wheat producing area in South-East Australia at 35.1°S and 142°E. The climate can be described as Mediterranean or semi-arid, typically prone to water limitation. This kind of low productive cropping systems resembles 15% of wheat growing regions in the world (Fischer et al., 2014). Here the mean annual rainfall (30-year average) lies at 320 mm with an average temperature of 18.3 C during the growing period. Normal wheat yields range between 1-3 ton/ha on grown on lower fertility sandy soils. Given the aforementioned, the Walpeup site denotes on of the driest and low productive agricultural sites where FACE experiments were conducted (Fitzgerald et al., 2016)

In the Australian site, the experiment was conducted on Yipi, which is a common spring wheat in the region whose phenological development is not characterised by any vernalization demands. Treatments differed between an early time of sowing (TOS1) and late time of sowing (TOS2). The later sowing time was applied with the goal to move the normal crop sowing period to mid-winter instead of the beginning of it in order to force phenological processes such as flowering and maturity to occur at hotter temperatures in late spring, simulating environmental conditions most likely present in a future climate. Furthermore, neither irrigation nor nitrogen fertilisers were additionally applied (Fitzgerald et al., 2016). Management practises are summarized in the table below (Table 4).

Table 4. *Management practises for the FACE experiment in Walpeup, Australia.*

Management	Units	2008 Wheat TOS1	2008 Wheat TOS2	2009 Wheat TOS1	2009 Wheat TOS2
Sowing	Date	19.05.08	30.06.08	14.05.09	20.07.09
N-fert. (H/L)	kg/ha	/	/	/	/
Final Harvest	Date	10.11.08	25.11.08	19.11.08	19.11.08
CO2 (ambient/elevated)	ppm	370/550	370/550	370/550	370/550

3.1.4 Selhausen, Germany

Measurements for evaluation of modelled GPP and NPP were obtained at a study side of 6.58 ha in Selhausen (50.9°N, 6.5°E). There an eddy covariance tower was installed in the middle of the study area. The climate is similar to the site in Braunschweig, which can be defined as temperate maritime having a yearly average temperature of 9.9°C and experiencing 698 mm of annual precipitation (Schmidt et al., 2012). Agricultural fields were managed according to conventional practises (Table 5). Given that data regarding timing and amount of fertiliser applied were provided, these parameters could be set for the model simulation, where 40% were applied halfway to anthesis and the remaining 60 % close to anthesis.

Table 5. *Management practises for the eddy covariance experiment in Selhausen, Germany.*

Management	Units	2007/2008 Wheat	2008/2009 Wheat
Sowing	Date	19.11.2007	18.10.2008
N-fert.	kg ha-1	196	160
Final Harvest	Date	06.08.2008	28.07.2009
CO2 (ambi.)	ppm	383	385

4 Results

The different simulations conducted in LPJ-GUESS for the locations mentioned under study sites are present below. This section starts with the results obtained for the model benchmark process and later elaborates on important findings in more detail that arose during the daily output analysis.

4.1 Model benchmark

The first step towards reaching the aim, was to create a model benchmark, which relates to running the model with the same conditions and treatments that were applied in the FACE experiment, as described under the study site section. Afterwards an analysis was carried out where observed data was compared to the modelled daily outputs. Going further than just investigating wheat yields, the response to elevated CO_2 was also dissected and placed into context.

4.1.1 Baseline CO_2 concentrations

The model's ability to simulate wheat yields observed under ambient CO_2 concentrations was tested by forming a baseline in the process. Below are the results for ambient (Fig. 1a) and elevated CO_2 (Fig. 1b) concentrations for all locations summarized, differentiated according to colour. If the simulated results are identical to the observations, the points would all fall onto the black line, indicating 100% agreement between modelled and observed yields. However, most obtained yields do not fall onto the 1:1 baseline but rather above, meaning that the model tends to underestimate yields in these locations. This underestimation is greatest for the US site (green), indicated by the larger distance to the 1:1 line, while for the German location (blue) the model seems to have a better fit. A similar trend can be observed for the elevated CO_2 concentration run, with the site in the US standing out the most (Fig. 1b).

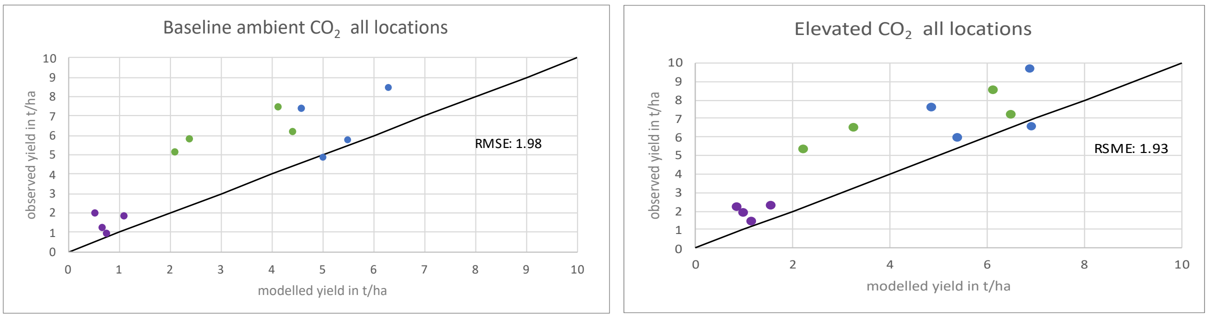

Figure 1. *Obtained wheat yields from LPJ-GUESS compared to observations. The left side (a) denotes ambient CO_2 and the right (b) elevated CO_2 concentrations. Colours stand for different locations with purple: Australia, green: USA and blue: Germany.*

Furthermore, the different responses to elevated CO_2 were analysed (Table 6), the strongest increase in gross primary productivity (GPP) can be found in Walpeup (35%), followed by Maricopa (33%) and lastly Braunschweig (17%). Similar increases occur for net primary production. Even though, the site in Braunschweig is modelled to have the lowest rise in productivity, there crop transpiration decreased the most after plants were exposed to enhanced CO_2 levels with 12%. In absolute terms, crops grown in Maricopa had the highest gain in GPP and NPP of 0.81 kg C/m^2yr and 0.5 kg C/m^2yr respectively.

Table 6. *Modelled CO_2 response for GPP, NPP and Transpiration for all locations. The left part denotes absolute differences between elevated and ambient conditions, the right part show the relative change from ambient conditions.*

	GPP [kgC/m2/yr]	NPP [kgC/m2/yr]	Transpiration [mm/yr]	GPP [%]	NPP [%]	Transpiration [%]
Braunschweig	0.32	0.23	-55.66	17	17.5	-12
Maricopa	0.81	0.50	-51.12	33	33.4	-5
Walpeup	0.16	0.11	-10.35	35	34	-7

4.1.2 Benchmark Braunschweig, Germany

When conducting a benchmark on the model to its ability on simulating wheat yields accordingly, the German site in Braunschweig performed well (Fig. 2a+b). Under ambient CO_2 concentration, the modelled yields have an average of 4.8 and 5.9 t/ha, for the low and high nitrogen input respectively, while observed yields range between 6 and 7 t/ha. Once CO_2 enrichment took place yields increased in the modelled version by 0.3 and 1 t/ha, compared to the production gain of 0.75 and 1.15 t/ha measured. This relates to a CO_2 response of 12%, in line with observational data showing a 15% response (Fig. 2b). Notably, the model underestimate yields in the growing period 2005 for all treatments, however the general patter of low and high nutrient input was captured.

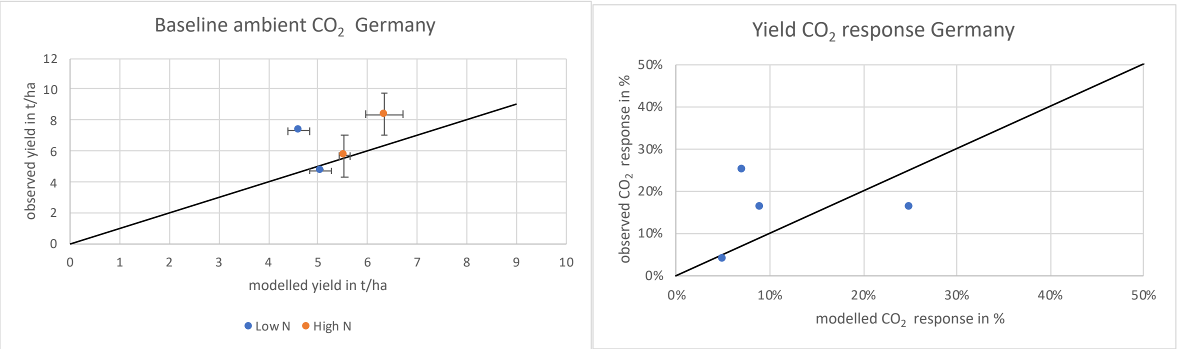

Figure 2. *Obtained wheats yield from LPJ-GUESS compared to observations in Braunschweig, Germany. The left side (a) denotes ambient CO_2 (with the standard error for observational data) and the right (b) the yield increase as response to elevated CO2 concentrations*

4.1.3 Benchmark Maricopa, USA

When investigating the model's performance for the FACE experimental site in Maricopa, USA, it becomes clear that yields are strongly underestimated (Fig. 3a). However, it is worth mentioning that LPJ-GUESS successfully encapsulates the variation between low and high nitrogen fertiliser input (Fig. 3a). Under ambient conditions the model simulates yields of 2.3 and 4.3 t/ha (low and high nitrogen application), while actual yields where higher with 5.4 and 6.8 t/ha. Exposure to elevated CO_2 led to production gain of 2 t/ha for both treatments, much higher than the 0.4 and 1 ton/ha increase obtained in field studies (Fig. 3b). The strong CO_2 response, resulted in an average response to enhanced CO_2 of 33%, on the other hand experimental data only showed a 12% rise.

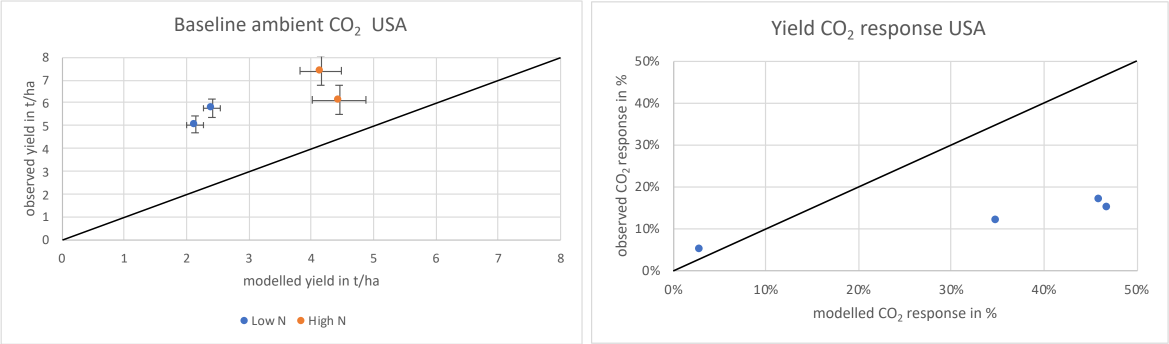

Figure 3. *Obtained wheat yields from LPJ-GUESS compared to observations in Maricopa, USA. The left side (a) denotes ambient CO_2 (with the standard error for observational data) and the right (b) the yield increase as response to elevated CO_2 concentrations.*

4.1.4 Benchmark Walpeup, Australia

Lastly the analysis was carried out for the Australia site in Walpeup. The same issue arises as it has previously in the American location, with underestimated yields (Fig. 4a). This is especially pronounced in the growing period 2009, where the modelled output for the late sowing time shows the highest deviation from observations for both ambient and elevated conditions (Fig. 4a). In general, this region is characterised by low productivity, further enhanced by the fact that neither irrigation nor additional fertilizer has been not applied. Observational data shows wheat production in the range of 0.9 to 1.9 t/ha, while the modelled simulations are lower with 0.6 to 1.1 t/ha. However, the modelled CO_2 response lies at 45%, which is the greatest increase obtain during the benchmark process but does not deviate substantially from the 40% reported in the field study (Fig. 4b).

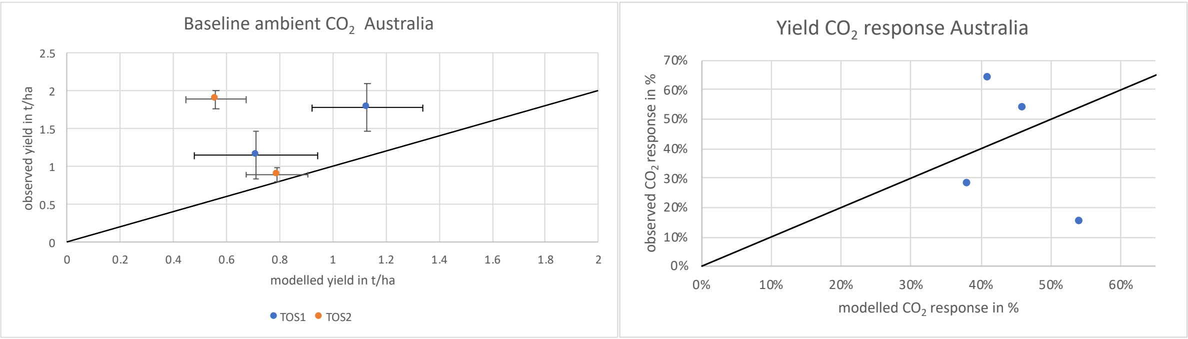

Figure 4. *Obtained wheat yields from LPJ-GUESS compared to observations in Walpeup, Australia. The left side (a) denotes ambient CO_2 (with error bars indicating the 4th standard deviation) and the right (b) the yield increase as response to elevated CO_2 concentrations*

4.2 Daily output evaluation

As has been shown above, the model is able to capture patterns accordingly corresponding to different nitrogen treatments but fails to accurately simulate observed yields. In order to gain knowledge on which process might explain or is responsible of this trend, daily outputs for NPP, LAI and water stress were analysed.

4.2.1 Leaf area index

A key parameter used to model plant process, including evaporation and canopy photosynthesis, is the leaf area index (LAI), which is defined as the ratio of one-side leaf area per unit horizontal ground are (Watson, 1947). It possesses a crucial role since it determines the size of the boundary area between biosphere and atmosphere, providing therefore an essential role in transfer of matter and energy between these spheres (Weiss et al., 2004).

The main finding was that development of leaf area index (LAI) is delayed. To illustrate this the growing period 1996 in Maricopa was examined, where the peak LAI of 3.77 and 5.48 m^2/m^2 for the low and high nitrogen treatment were measured 87 days after sowing (Fig. 5). However, the model's daily output showed that the maximum LAI value is not reached until 155 days after sowing, which translates to a total delay of 68 days. Furthermore, it can be noted that not only is the modelled LAI higher with 4.3 and 6.6 m^2/m^2, but more carbon gets allocated to the leaves for a longer time duration.

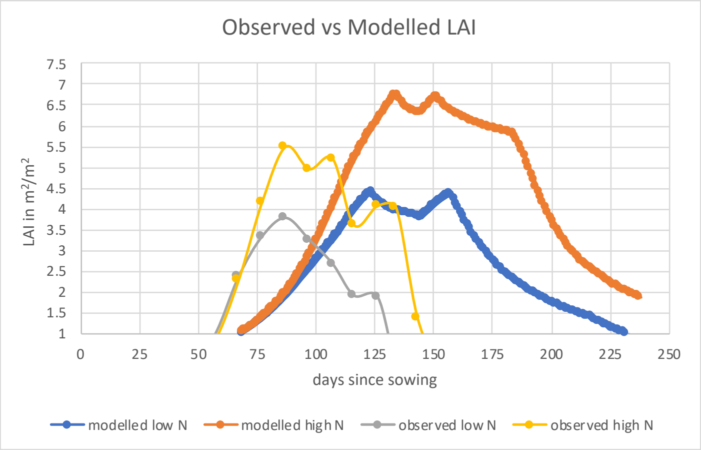

Figure 5. *Obtained LAI from LPJ-GUESS compared to observations in Maricopa, USA during growing period 1996.*

The same patterns can be observed in the other two model runs, where the delay is especially pronounced in Germany (Fig. 6). Under elevated CO_2 conditions, field data collected in Germany measured an LAI of 2.95 m^2/m^2 during anthesis, while in the model this value is not reached until 200 days after sowing. Lower LAI values can be found in the Australian side, where a threshold ratio of 2 m^2/m^2 exists. From the obtained daily outputs and the observational data, it becomes clear that there is a consistent delay in LAI development through all runs.

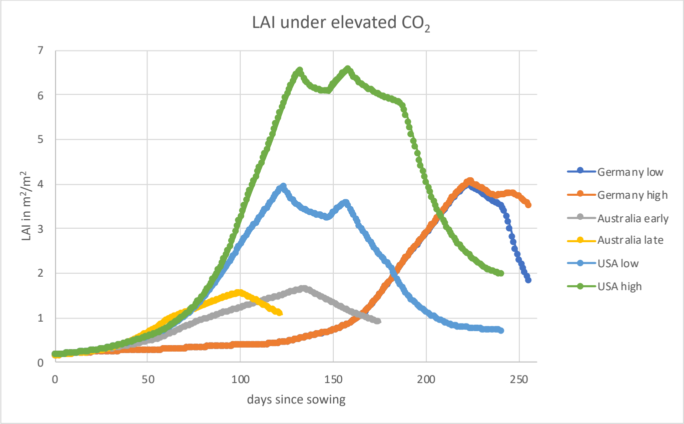

Figure 6. *Obtained LAI from LPJ-GUESS for all 3 locations under elevated CO$_2$*

4.2.2 Water stress

Another possible explanation for the underestimated yields might be water stress early in the growing period, preventing leaf carbon from accumulating, which ultimately leads to a delay in LAI development. For this purpose, daily outputs of water stress were investigated.

The results showed that this stressor is not present in the beginning of the growing season but starts to build up in magnitude once LAI started to rise, as can be seen in the Australian site (Fig. 7). In Walpeup strong water stress occurs for both the early and late sowing time. During the growing period, water stress reaches values of up to 0.1, on a scale from 0 to 1, where 1 denotes no presence of water stress, while 0 is complete exposure. A similar pattern with enhanced water stress after LAI development can be observed at the US site, but to a lower degree (Fig. A1). However, the German site is not affected by water stress at any point during the crop growth, which is the reason why results from this location are excluded. As water stress does not impact the crops in the beginning of their development nor does it impact wheat growing at the German site, it cannot account for the delayed LAI.

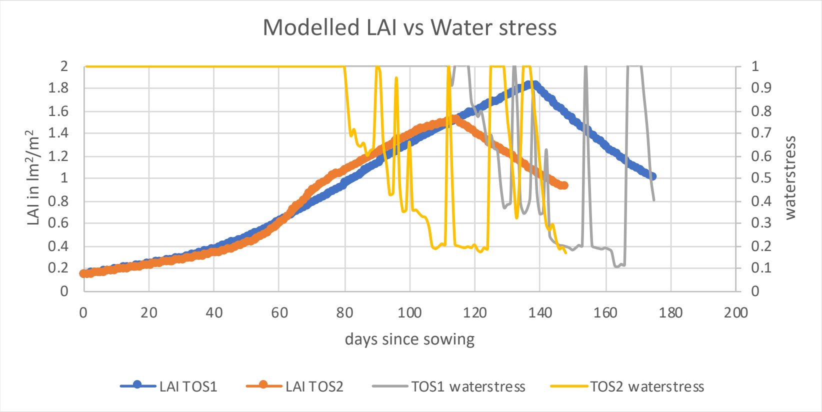

Figure 7. *Obtained LAI and water stress from LPJ-GUESS under elevated CO$_2$ during growing season 2008 in Walpeup, Australia.*

Furthermore, at the Australian site difference in water stress can be found between the different CO$_2$ treatments, where reductions can be observed under elevated concentrations (Fig. 8). Days where no changes occurred were removed to aid the presentation. While most days during the growing season experience water stress reductions below 0.06, a considerable amount of days improves to a greater degree with values between 0.10 and 0.26. Water stress tends to advance earlier in the growth stage for the crops planted at a later point in time, while the opposite can be observed for the early sowing time. No clear differentiation between ambient and elevated water stress levels can be made for Maricopa, as most of the days fall below the 0.05 threshold.

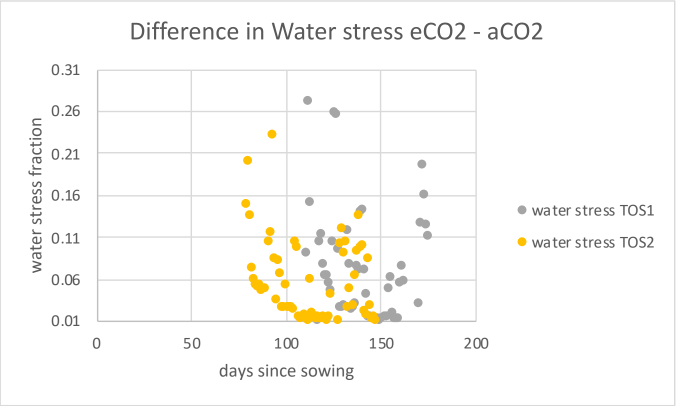

Figure 8. *Difference in water stress between elevated and ambient CO_2 during growing season 1996 in Maricopa, USA.*

4.2.3 Modelled net primary productivity

To test whether the delayed LAI originates from wrongly modelled net primary production (NPP) in the first place, a winter wheat cropping system in western Germany was analysed. There measurements of GPP, NPP and autotrophic respiration (R_{AUT}) were gathered with the help of a eddy covariance flux tower and evaluated against simulated results (Schmidt et al., 2012).

Firstly, the modelled LAI development for both growing seasons 2007/8 and 2008/9 are depicted below (Fig. 9), which follows a similar trajectory to the previous simulated runs. In the field study both years reach their maximum LAI of 5.6 and 5.9 m^2/m^2 in the beginning of May (Schmidt et al., 2012), while in the model a maximum of around 3.6 m^2/m^2 occurred towards mid to end of June, 225 and 250 days after sowing (Fig. 9). This translates to a delay in LAI of 1.5 months.

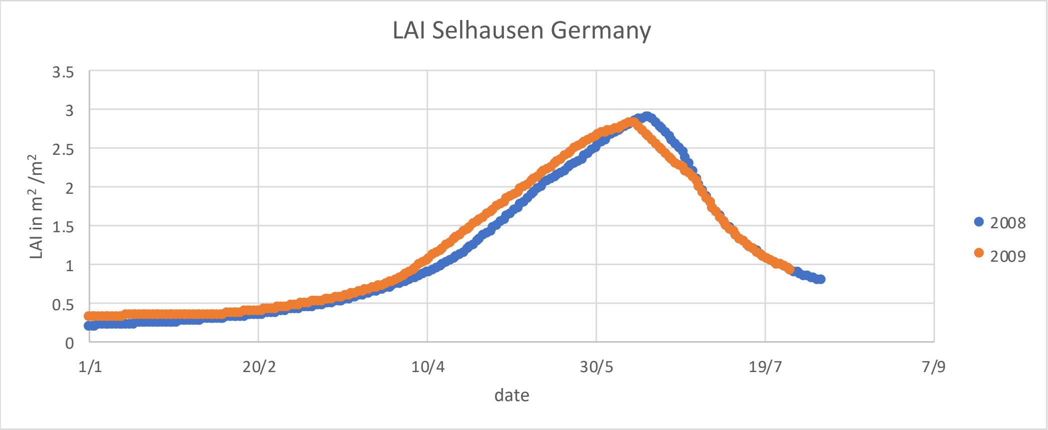

Figure 9. *Modelled LAI development under ambient CO_2 during two growing seasons in Selhausen, Germany. Not visualized are the months November and December.*

When comparing the modelled GPP and NPP to observational data, it becomes apparent that LPJ-GUESS is not able to correctly represent GPP, NPP and R_{AUT} (Table 4). GPP is underestimated in both years, with 0.97 and 0.83 kg C/m^{2}yr taken up by the vegetation, while measurements show uptakes that are 37% higher. However, NPP on the other hand is overestimated showing a 25% increase compared to observed data, which is especially pronounced in the growing period 2007/8 where NPP fluxes have a 35% increase. The greatest variation can be found in autotrophic respiration, whose participation is of a low degree with 0.28 kg C/m^{2}yr and 0.24 kg C/m^{2}yr, while observed values are almost three times the amount.

Table 7. *Modelled and observed GPP, NPP and R_{AUT} under ambient CO_2 in Selhausen, Germany.*

	Growing season	GPP [kg C/m2yr]	NPP [kg C/m2yr]	RAUT [kg C/m2yr]
modelled	2007/8	0.97	0.69	0.28
	2008/9	0.83	0.58	0.24
observed	2007/8	1.34	0.45	0.89
	2008/9	1.12	0.50	0.62

There seems to be however an offset between observed and modelled GPP and NPP, which was especially pronounced in the beginning of the growing period, where the simulated fluxes only indicate low productivity. Daily outputs of NPP reveal that most of the productivity occurs towards the end of crop growth, with 37% of total productivity occurring in the last 15% of the growing season, and 57% of NPP accumulates within the last 23% (Fig. 10). The highest fluxes of NPP are simulated to occur in June and July of reaching values around 8 g C/m^{2}d.

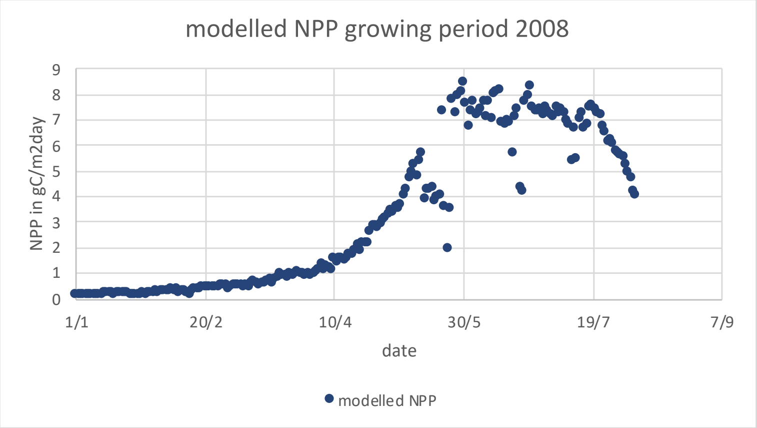

Figure 10. *Obtained NPP [gC/m^{2}d] from LPJ-GUESS under ambient CO_2 Selhausen, 2008. Not visualized are the months November and December due to low productivity.*

5 Discussion

In the following sections the obtain results will be dissected and placed into a larger context regarding implications for future crop yield models.

5.1 Benchmark

When conducting the benchmark process LPJ-GUESS tended to underestimate yields compared to observational data (Fig 1-4). This underestimated occurred for both ambient and elevated CO_2 runs. Furthermore, the model had more difficulties in simulating yields correctly in drier climatic regimes, such as Maricopa and Walpeup given that the deviation to observational data is the strongest. On the other hand, the model appears to be more calibrated for temperate ecosystems, as the German site in Braunschweig gave the best agreement with field data. Nonetheless of the shortcoming, LPJ-GUESS was able to simulate crop responses due to elevated CO_2 well for the Germany and Australian sites. Studies employed at these locations showed a CO_2 response of 15% and 40% in Germany and Australia. The outlier was the American site were the model failed to firstly simulate yields under both CO_2 treatments but also the CO_2 response was modelled too high with 33 % instead of 12%, which translates to yield gains of 2 ton/ha.

This might be explained by the fact that crop models generally shown to have a harder time depicting yields correctly for certain ecosystems, including drier environments, possibly due to the difficulty in representing the complicated interactions between higher temperatures, heat and water stress and elevated CO_2 all at once (McGrath & Lobell, 2013). Lack of experiments where the interplay of these variables with elevated CO_2 has not been examined in detail might portray one of the reasons for this challenge (Asseng et al., 2004; Parry et al., 2004).

Previous research has found a correlation between yield increases due to elevated CO_2 and regional productivity, where low productive systems respond the strongest (Broberg et al., 2019). This greater rise in grain yields observed in crops growing in drier or water stressed environments can be attributed to improvements in water use efficiency (Kimball et al., 2002). In fact, the driest and most water stress cropping system analysed in this study, namely site in Walpeup, showed the greatest yield increases under elevated CO_2 with a modelled response of 45% in LPJ-GUESS. While in observational data at the FACE facility a mean yield increase of 40% could be measured, with some treatments simulated a CO_2 response of up to 70 % (Fitzgerald et al., 2016).

On the other hand, regions characterised by high yields under ambient CO_2 concentrations, did not experience substantial yield increases after enrichment treatment. Hinting on the existence of a negative link between site productivity and yield gain (Broberg et al., 2019). These findings are in hand with the modelled results obtained at the German site, where grain yields were already high with an average of 5.5 t/ha under ambient CO_2 concentrations, and CO_2 enrichment led to the lowest simulated grain yield rise of 12%.

A similar rise in grain yields of 19% was achieved during a previous modelling study conducted by Olin et al. (2015), which evaluated the performance of an earlier LPJ-GUESS version in simulating cereal yields at the same FACE location close to Braunschweig. However, there acquired yields under ambient CO_2 concentrations were modelled to be higher compared to values obtained in this study. The differences in yields relative to Olin et al. (2015) range between 2 and 3 ton/ha for the low and high nitrogen treatments respectively. This deviation could be explained by the fact that this study solely focused on modelling the growing periods where winter wheat was sown, while Olin et al. (2015) included the impact of CO_2 on winter barley. Another deviation can be found in the climate data set used and the fact that parameters for wheat were updated in this study, potentially explaining why similar inputs lead to different results.

Another study conducted by Smith et al., 2014 investigated LPJ-GUESS performance in simulating forest productivity globally under elevated CO_2 levels. Productivity increase in NPP appears to have a spatial characteristic, where NPP gain tends to be lower at higher latitudes but rises when approaching tropical environments. This small percentage rise in the higher latitudes might be attributed to inadequate nitrogen availability, since colder climatic conditions slow down nitrogen mineralisation and its fixating. Thus, giving space to soils with low nitrogen content, which might not be capable to support the canopy's larger requirements, as it becomes less CO_2 limited (Smith et al 2014). Given that firstly, none of the investigated locations in this study were situated North of Braunschweig in Germany and secondly, cropping systems tend to rely on fertiliser application, it would be difficult to assess whether nitrogen limitation caused by colder climate might be responsible for lower crop productivity. This limitation might apply solely for natural vegetation, as manually applied fertilizers would buffer the slower turnover of natural nitrogen sources.

To add on Smith et al. (2014) attributed the simulated increase in forest NPP of 40-50%, in climate regimes described as warm temperate to subtropical, to a synergistic effect on photosynthesis and autotrophic respiration, which would lead to enhanced carbon use efficiency. Furthermore, it was noted that the elevated CO_2 levels occurring during the FACE experiments might increases photosynthetic rates, which consequently leads to a higher carbon presence in the newly acquired biomass compared to its nitrogen content. Nitrogen amounts in plant tissue determine respiration rate; with less nitrogen present respiration rates are weakened, which aids the intensification of NPP, proportionate to the GPP gain (Smith et al 2014.)

5.2 Daily output evaluation

From the models' daily outputs, it became apparent that LAI development is delayed and often not depicted in the correct way (Fig.5-6). To illustrate this behaviour observed LAI and modelled LAI were analysed in Maricopa during the growing season 1995/6 and a slowing down of progression by 1.5 months has been noted in the comparison process (Fig. 5). While the model successfully simulated the correct pattern, the LAI values were higher, and more carbon seemed to have been allocated to the leaves for a longer time period due to the larger area present under the curve. The delay of 1.5 months is consistent throughout other modelled runs as well, as results from a comparison study conducted with other experimental data, such as LAI evolution measured at a cropping system in Selhausen showed the same behaviour (Schmidt et al., 2012).

Since water stress early in the growing season might reduce carbon accumulation, daily outputs were analysed for this purpose. Although, the results do not suggest the presence of this stressor in the beginning of crop growth to be responsible for delayed LAI development, reductions of water stress between the different CO_2 treatments (Fig. 8) took place. For example, in Walpeup this might be one of the reasons explaining why crops grown in that environment had the strongest CO_2 response of 45% modelled. Given the fact that water stress between ambient and elevated CO_2 treatments did only improve to a lower degree in Maricopa and no change was observed in Braunschweig, this hints on the fact that enhanced water use efficiency might be at play, which caused increased biomass accumulation and grain yield. In fact, water use efficiency substantially increased after exposure to elevated CO_2 with a rise of 34% in Germany, 41 % in the US and 43 % in Australia. This can be further attributed to the fact, that the German site had the strongest decline in transpiration, followed by the US site (Table 6).

During the comparison of modelled and measured crop processes such as GPP and NPP it was found that neither GPP nor NPP are accurately depicted in the model (Table 7). Moreover, the NPP values were overestimated by around 25%; due to the fact that biomass development and carbon assimilation in crop tissues solely depend on NPP, the GPP underestimation cannot be accounted for the delay in LAI nor lower yields. Thus, the issue regarding the delayed LAI development is mostly an error of mechanical nature within the model.

Furthermore, the gap between observed and modelled GPP implies a bias in the model, where firstly crops do not respire as much as they do compared to field measurements but also productivity is simulated to start off slowed down in the beginning of the modelled growing period and starts to accelerate rather fast towards the end. Thus, when trying to model crops growing in a future climate exposed to both elevated CO_2 and climate change interactions, which included for example increased temperatures (Cossani & Reynolds, 2012; Easterling & Apps, 2005), yields might even get more underestimated. This underestimation would occur, as most of the biomass will be modelled to accumulate at the end of the growing period when temperature are hotter and less favourable for crop development. This yield underestimating might be even more enhanced in drier and water limited environments, when drought issues arise, especially if these are present at the end of the growing season, where most modelled NPP production takes place, leading to further complications in successful yield simulations. Given that extreme weather events are projected to become more frequent, which in turn not only imposes damage to crops physically but also influences timing in their development and growth (Powell & Reinhard, 2016), it will be essential to resolve the aforementioned issues, in order to be able to provide the best model yield estimates.

5.3 Outlook

Another aspect to consider is that the investigated enriched level of CO_2 of 550 ppm, is on the lower spectrum of how future atmospheric concentrations might look like and another study suggested a positive CO_2 responses until concentrations reach 600 ppm, whereas a leveling off might occur beyond this threshold (Broberg et al., 2019). Moreover, it will become more important in the upcoming future to administer a variety of FACE experiments under higher CO_2 concentrations with the goal to analyse crop response for data acquisition which can be used in model validation and tuning process.

5.4 Limitations

A main limitation when conducting all the model runs in LPJ-GUESS has been that the climatic data used, was based on interpolated data instead of utilising climate conditions measured at stations close to the FACE facilities due to time constraints on setting up the LPJ-GUESS simulations. Thus, acquiring observational climatic data would lead to a more elaborate study, possibly providing enhanced results with stronger agreement to field studies.

Furthermore, lacking information regarding timing and amount of fertilizer application, might have led to the difference in simulated versus observed yields at the German site and generalisations had to be made. Generalisations are never as good of an estimate as actual measurements, highlighting the importance for experimentalist to include data regarding specific treatments applied as it impacts simulated results. Moreover, the availability of detailed observational data is essential in order to simulate yields correctly and validate models.

Another limiting factor to consider is that the option to simulate different water treatments is not easily applicable in the model, as the irrigated management feature assumes perfect water availability and an in-between state is not achievable without manipulating climatic data.

During the evaluation whether estimated GPP and NPP in the model were not depicted accordingly, finding studies conducted on winter wheat in similar environments as the previous locations was challenging, ultimately resulting in only one comparison. When conducting studies similar to this one, it would be important to be able to compare local observed GPP and NPP, to decipher whether one of the fluxes gets incorrectly simulated in the first place, resulting in underestimated or overestimated yields or if other processes are not modelled accordingly. Therefore, it would be beneficial when conducting FACE experiments to also invest in the installation of eddy covariance flux tower, as it can give direct insight on potential reasons behind modelling issues and could also act as another parameter used for model validation.

6 Conclusion

During the evaluation of LPJ-GUESS performance in simulating yields, shortcomings were noted namely in underestimation of yields, which occurred both under ambient and elevated CO_2 conditions. However, it was found that the CO_2 response modelled was within reason and LPJ-GUESS tends to perform better in temperate climatic regimes compared to drylands. Further enhanced by the fact that the best agreement between observed and modelled yield was found at the German side in Braunschweig, while the strongest deviations occurred at the US side. When investigating the reason behind yield underestimations, another major finding has been the delayed leaf area index (LAI) development. After further investigation of the relationship between water stress and LAI, it was concluded that as water stress is not present in the beginning of the growing season, it cannot be attributed to the offset in LAI development. As final part of the analysis daily outputs for NPP were compared to ground data obtained from a study side in Selenhausen, and the results showed that the simulated NPP is overestimated by 25%, contrarily the model tends to underestimate GPP. Since LAI development is moderated by NPP, the offset in its build up does not take place due to underestimation of simulated NPP values and is therefore most likely a mechanistic error within the model.

Once a crop model is able to simulate the response of wheat to elevated CO_2 accordingly, it might be appropriate to utilise this kind of model to perform estimates of future yields. Thus, the issue regarding the underestimating yields needs to be solved first, in order to be able to utilise this model for future studies. Moreover, the bias found within the model might make successful yield estimates for future climate scenarios more challenging, as it potentially introduces even lower yield simulations due to the enhanced interactions of elevated CO_2, increased temperature, and drought at the end of the growing period, where most of the biomass is accumulating.

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Appendix A

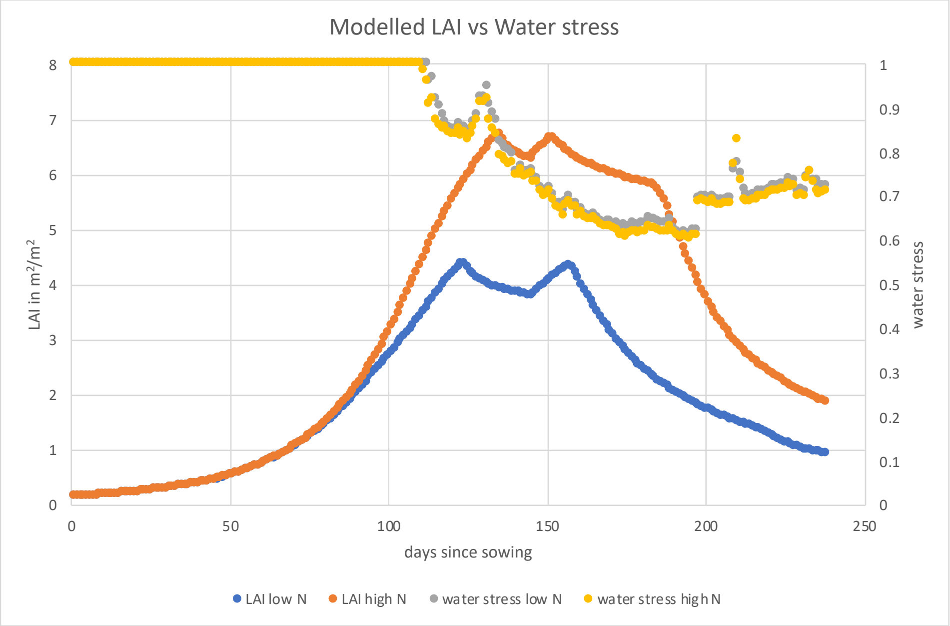

Figure A1. *Obtained LAI and water stress from LPJ-GUESS for under elevated CO_2 Maricopa, USA.*

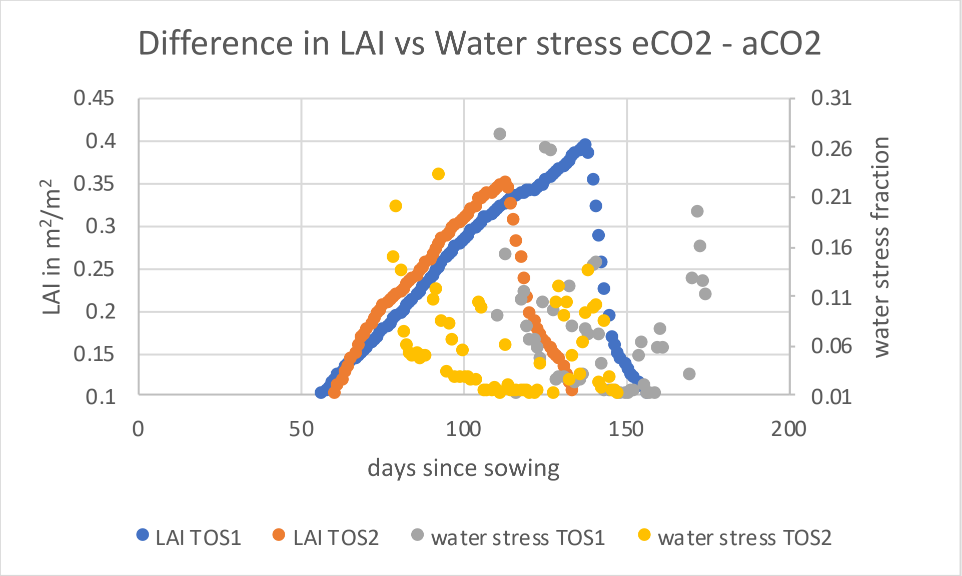

Figure A2. *Obtained LAI and water stress from LPJ-GUESS for elevated -ambient conditions Walpeup, Australia*