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Relevance of feedbacks between water availability and crop systems using a coupled hydrology – crop growth model

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Abstract

Individual hydrological and crop growth models often oversimplify underlying processes, reducing the accuracy of both simulated hydrology and crop growth dynamics. While crop models tend to generalize soil moisture processes, most hydrological models commonly use constant vegetation parameters and prescribed phenologies, neglecting the dynamic nature of crop growth. Despite some studies that have coupled hydrological and crop models, a limited understanding exists regarding the feedbacks between hydrology and crop growth. Our objective is to quantify the feedback between crop systems and hydrology on a fine-grained spatio-temporal level. To this end, the PCR-GLOBWB 2 hydrological model was coupled with the WOFOST crop growth model to quantify both the one-way and two-way interactions between hydrology and crop growth on a daily timestep and at 5 arc minutes (~10 km) resolution. Our study spans the Contiguous United States (CONUS) region and covers the period from 1979 to 2019, allowing a comprehensive evaluation of the feedback between hydrology and crop growth dynamics. We compare individual (stand-alone) as well as one-way and two-way coupled WOFOST and PCR-GLOBWB 2 model runs and evaluate the average crop yield and its interannual variability for rainfed and irrigated crops as well as simulated irrigation water withdrawal for maize, wheat and soybean. Our results reveal distinct patterns in the temporal and spatial variation of crop yield depending on the included interactions between hydrology and crop systems. Evaluating the model results against reported yield and water use data demonstrates the efficacy of the coupled framework in replicating observed irrigated and rainfed crop yields. Our results show that two-way coupling, with its dynamic feedback mechanisms, outperforms one-way coupling for rainfed crops. This improved performance stems from the feedback of WOFOST crop phenology to the crop parameters in the hydrological model. Our results suggest that when crop models are combined

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with hydrological models, a two-way coupling is needed to capture the impact of interannual climate variability on food production.

1 Introduction

Global trends in population and economic growth are expected to increase the demand for water, food, and energy, threatening the sustainable and equitable use of natural resources (Sophocleous, 2004; Tompkins and Adger, 2004). Water as a resource plays a crucial role in crop growth, cooling of thermoelectric plants, hydropower generation, and covering domestic and industrial demand. Water, therefore, is an essential resource at the core of the Water-Energy-Food-Ecosystem (WEFE) nexus. Currently, 70% of total global freshwater withdrawals are accounted for by agriculture, making it the largest water user among all sectors (Dubois, 2011). The Food and Agriculture Organization (FAO) of the United Nations estimated that the demand for water and food resources will likely increase by 50% by 2050 compared to 2015 (IRENA, 2015; Corona-López et al., 2021). The increasing demand for water and food will likely have negative impacts on the environment and will inhibit socio-economic development if a gap opens between growing water demand and water availability.

The critical interplay between hydrology and crop growth becomes evident during hydroclimatic extremes (e.g. droughts, heatwaves), as rising demands coincide with potential declines in both water resources and food production (crop yield) (Jackson et al., 2021). In addressing the complexities associated with these challenges, studies by Jägermeyr et al. (2017), utilizing a dynamic vegetation model (LPJmL), evaluated achievable irrigated crop production under sustainable water management. Their findings revealed that 41% of global water use currently compromises environmental flow requirements crucial for river ecosystems, potentially leading to losses in irrigated croplands. Concurrently, research by Vörösmarty et al. (2000) and Leclère et al., (2014) projects the impacts of climate change on global agricultural systems, foreseeing an increase in irrigated areas in the future, underscoring the necessity for significant investments in irrigation, energy, and water resource management.

Biophysical process-based models, as highlighted by Siad et al., (2019) and Zhang et al., (2021), are instrumental in understanding the intricate relationship between hydrology and crop growth, particularly in response to changing hydroclimatic conditions. Considering factors like irrigation water use and soil-groundwater dynamics, these models explore how meteorological

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events influence water availability for crops, as well as the impacts of diminished growth and premature senescence on hydrology through effects on root water uptake and evapotranspiration. This understanding becomes crucial when assessed at the regional to global scale, where local deficits can have cascading consequences for both water and food security.

In the context of studying the impact of climate change and variability on crop yields, aside from biophysical models, numerous crop models have been employed. However, these models often incorporate a simplified soil-water balance (Zhang et al., 2021) that overlooks local hydrological processes and often do not account for water use for irrigation and non-agricultural sectors. Conversely, most hydrological models simplify or neglect the effects of land cover, phenology and vegetation changes on hydrological fluxes and the state of available water resources (Tsarouchi et al., 2014). These simplifications arise due to computational expediency, disparities in process scales between hydrology at the river basin level and crop yield at the field level, incomplete understanding of the other domain by model developers, or because of epistemological uncertainty (Siad et al. 2019; McMillan et al., 2018; Shafiei et al. 2014). Recognizing the strengths of both crop models and global hydrological models, a coupling allows for the exploration of dynamic crop growth's influence on hydrology and water use and the incorporation of accurate spatio-temporal variations in hydrological fluxes, including water use, in estimates of crop yield.

Noteworthy efforts by Droppers et al. (2021) have successfully coupled hydrological and crop models, primarily focusing on achieving attainable crop production. However, these efforts were conducted at half-degree (~50 km) spatial resolution and focused on long-term average crop yield. They therefore fall short in exploring the aspects of fine-scale spatiotemporal variability in particular as a result of interannual climate variability. Other recent efforts to couple crop growth models and global hydrological models (Jägermeyr et al., 2017) predominantly focus on assessing yield under different scenarios or adaptation measures. However, limited work focused on delving into how two-way interactions and feedback mechanisms between crop growth and hydrological systems operate.

In addition, integrated assessment models have been instrumental in studying the combined effects of climate change and socio-economic developments on crop yield and water resources at a large scale. Typically, these models operate on a macro-regional level (Easterling, 1997) and use annual (or 5 to 10 yearly timesteps), neglecting the impacts of inter- and intra-annual variability and particularly short-term hydroclimatic extremes. Furthermore, integrated

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assessment models often adopt an optimization modelling approach, making them less suitable for studying the effects of hydroclimatic extremes (Ewert et al., 2015).

Another class of efforts to link water to crop production are water-food nexus studies, that, however, tend to concentrate on local linkages or provide qualitative descriptions of existing connections (Momblanch et al., 2019). For instance, a recent review of water-food nexus studies focusing on the contiguous United States (CONUS), shows that such studies focus mainly on water security indicators (Veettil et al., 2022) or climate variability impacts on crop yields (Huang et al., 2021). However, knowledge gaps persist, as water and food resources are often evaluated separately (Corona-López et al., 2021), exploring allocations through an optimization model (Mortada et al., 2018) that lacks spatiotemporal variability considerations. Notably, there is a lack of effort to understand the interactions between hydrology and crop growth. Further research is needed to bridge these gaps and enhance our understanding of the dynamic and interlinked processes shaping the water-food nexus.

To address this knowledge gap, our objective is, therefore, to quantify the feedback between crop growth and hydrology. Although eventually global scale in scope, we limit this analysis to the Contiguous United States (CONUS) region, to keep the analysis tractable and because CONUS has detailed information on yearly crop production and water use.

CONUS is a major producer and contributor to the global production of three primary crops: maize, soybean, and wheat. These crops were selected due to their substantial impact on the agricultural landscape and their pivotal role in shaping global food production trends. The CONUS serves as an ideal study area owing to its extensive availability of relevant data, particularly on agricultural statistics and irrigation water withdrawals, which can provide a basis for analysis and model evaluation. Additionally, the CONUS region exhibits diverse climatic and geographic conditions, contributing to a better understanding of crop and water system dynamics and their responses to various environmental factors.

To this end, we developed a coupled global hydrological-crop growth model framework to answer questions related to 1) the impacts of irrigation and hydrology on crop growth; 2) the feedbacks of crop growth on the hydrological system when accounting for interannual variability; and 3) the importance of the two-way coupling between hydrology and crop growth to provide realistic water resources and crop yield simulations. By delving into these aspects, we aim to contribute valuable insights into the feedback processes between hydrology and crop growth, thereby addressing the current research gap in a more comprehensive manner.

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To address this, the PCR-GLOBWB 2 hydrological model (Sutanudjaja et al., 2018) is coupled to the WOFOST crop model (de Wit et al., 2019) at a daily timestep and at 5 arc minutes (~10 km) spatial resolution applied to CONUS (section 2.1). First, a one-way coupling is established to evaluate the effect of the simulated water availability of PCR-GLOBWB 2 for rainfed and irrigated crop growth in WOFOST (section 2.1; section 2.2.1). In addition, a two-way coupling is established in which, additional to passing water availability from PCR-GLOBWB 2 to WOFOST, the crop phenology of WOFOST in terms of actual evapotranspiration, leaf area index and rooting depth is fed back into PCR-GLOBWB 2 (section 2.1, 2.2.2;). Furthermore, individual WOFOST and coupled one-way and two-way model runs were compared to evaluate the impacts of feedbacks on crop yield and irrigation water use (section 2.3). The results of these simulations are compared with and evaluated against reported yield statistics and reported annual irrigation withdrawals to assess their validity (section 2.4; section 3). In the end, we elaborate on the uncertainties, strengths, and usability of our coupled model framework for studying the water-food nexus under global change (section 4).

2 Methods

2.1 Coupled PCR-GLOBWB 2-WOFOST model framework

A new fully coupled PCR-GLOBWB 2 - WOFOST model framework is developed to include the feedbacks between crop growth and hydrology. Here, we included both a one-way and two-way coupling between the PCR-GLOBWB 2 global hydrology and water resources model (Sutanudjaja et al., 2018) and the WOFOST crop growth model (de Wit et al., 2019). This coupled framework was then used to quantify the impacts of included feedbacks between hydrology and crop growth on a daily timestep and 5 arcminutes resolution for CONUS. The following (sub)sections provide a description of the PCR-GLOBWB 2 and WOFOST models and modules used (2.1), the model coupling setup (2.2), model coupling simulation experiments and parametrization (2.3), validation of crop yield and of irrigation water use (2.4).

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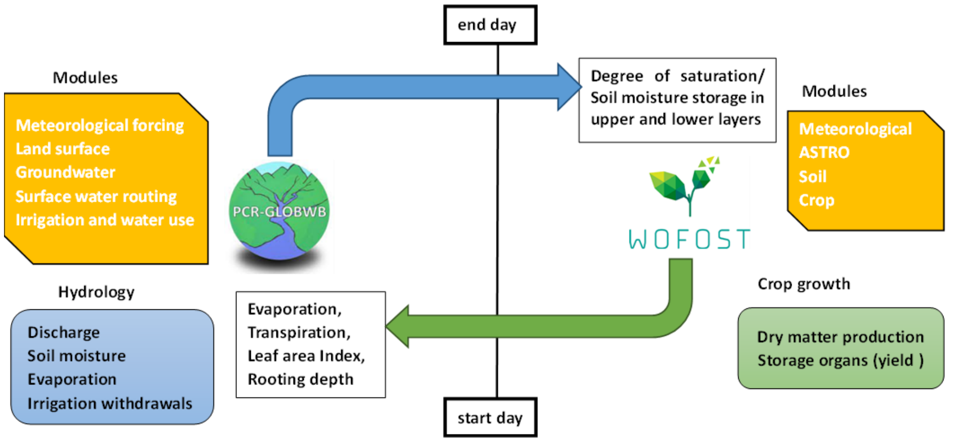

Figure 1: The coupled model framework of the PCR-GLOBWB 2 hydrology and water resources model and the WOFOST crop growth model. The blue arrow represents the one-way coupling from PCR-GLOBWB 2 to WOFOST and the variables that are exchanged; the green arrow is added in case the full two-way coupling is considered. At the start of the day, WOFOST computes evapotranspiration, leaf area index, and rooting depth that is used by PCR-GLOBWB 2 to compute soil moisture status. At the end of the day, soil moisture storage in the upper and lower layers from PCR-GLOBWB 2 is fed to WOFOST to compute crop growth for the next day.

PCR-GLOBWB 2

The PCRaster Global Water Balance (PCR-GLOBWB 2) model (Sutanudjaja et al., 2018) is a global hydrology and water resource model developed at Utrecht University. This model operates on a latitude-longitude grid for which it simulates fluxes and stores of the terrestrial hydrological cycle with a daily resolution and dynamically includes anthropogenic impacts such as man-made reservoirs and sectoral water demands, water withdrawals, consumptive water use, and return flows. The PCR-GLOBWB 2 model currently consists of five main hydrological modules encompassing meteorological forcing, land surface, groundwater, surface water, irrigation and water use (Fig. 1).

The PCR-GLOBWB 2 meteorological forcing uses a gridded time series of temperature and precipitation as input. More information on input datasets is provided in supplementary I. Reference potential evaporation is computed within the model using Hamon's (1963) method. The resulting reference potential evaporation is then employed in the land surface module to calculate the crop-specific land cover potential evaporation. Separate soil conditions are specified for each land cover type, with vegetative and soil properties varying accordingly for each grid cell and land cover type. The groundwater and surface water modules simulate the fluxes and stores of groundwater and surface water, respectively. The irrigation and water use module focuses on simulating water demand, withdrawals, consumption, and return flows. For

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a more detailed understanding of each module, we refer to the comprehensive description provided by Sutanudjaja et al. (2018).

WOFOST

WOFOST (WOrld FOod STudies) is a crop simulation model developed at Wageningen 'School of De Wit', in the Netherlands, designed to quantitatively analyze the crop growth and potential production of annual field crops at the field scale (Supit et al., 1994). WOFOST employs a fixed time step of one day to simulate crop growth based on eco-physiological processes such as phenological development and growth (de Wit et al., 2019). WOFOST has found extensive application in assessing the impacts of climate change and management strategies on crop growth and yield at local to global scales.

The WOFOST crop model comprises of four modules: weather, crop, astro and soil (Fig. 1). The WOFOST modules simulate a range of processes, including phenological development, CO_2 assimilation, leaf development, light interception, transpiration, respiration, root growth, assimilated partitioning to the various organs and the formation of dry matter. The model's output includes simulated crop biomass total, crop yield and variables such as leaf area and crop water use.

2.2 Model coupling setup

The PCR-GLOBWB 2 - WOFOST coupled model framework integrates hydrological and crop models through both one-way and two-way couplings, as illustrated in Fig. 1. This model coupling aims to assess the intricate interactions between hydrology and crop growth under different agricultural conditions, specifically irrigated and rainfed settings. The one-way coupling examines the impact of water availability on crop growth, while the two-way coupling incorporates the exchange of soil moisture status and hydrological parameters and fluxes based on crop status.

The online coupling process occurs seamlessly at each time step, facilitating dynamic interactions between WOFOST and PCR-GLOBWB 2 and limiting I/O-related computation times. To achieve this integration, we utilized the Basic Model Interface (BMI) (Hutton et al., 2020; Peckham et al., 2013), which is particularly valuable as WOFOST and PCR-GLOBWB 2 are written in different programming languages (C and PCRaster-Python, respectively). The decision to use BMI was driven by its non-interfering nature, ensuring no code entanglement and facilitating seamless connection between the models. BMI functions act as a bridge,

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enabling direct variable exchange between WOFOST and PCR-GLOBWB 2 without modifying their source code. This non-invasive approach ensures a flexible and robust coupling framework, allowing for continuous model development without interruptions. Integrating BMI functions into both models provides a set of functions for retrieving or altering model variables, enhancing adaptability and efficiency. The schematization of the workflow of the coupled PCR-GLOBWB 2 - WOFOST model framework can be seen in Supplementary Information II Fig. S1. Further details on BMI functions used for the development of the coupled PCR-GLOBWB 2 – WOFOST model framework are available in supplementary II.

2.2.1 One-way coupling

In the one-way coupling, information on soil hydrology is passed from PCR-GLOBWB 2 to WOFOST (Fig 1). Here, PCR-GLOBWB 2 simulates soil moisture content for every day and the soil water storage is simulated separately for each land cover type. Consequently, WOFOST receives the soil moisture content from PCR-GLOBWB 2 as input, with generally higher values of soil moisture for irrigated crops than of nearby rainfed crops. WOFOST then simulates the crop yield based on the simulated soil moisture content and the same meteorological inputs as PCR-GLOBWB 2 uses.

The combined model framework captures the impact of hydroclimatic conditions by assessing water stress and heat stress. Water stress, influenced by soil moisture levels derived from PCR-GLOBWB 2, affects various processes in WOFOST such as a reduction in the leaf area, a decrease in the assimilation of biomass (growth), changes in the partitioning of biomass, and an increase in various plant organs of senescence (ageing processes). Elevated temperatures have varying effects across different stages of crop development. They can accelerate crop growth by promoting faster accumulation of Growing Degree Days, which are essential for determining crop maturity. However, prolonged exposure to high temperatures can also induce heat stress, adversely impacting crop health and potentially shortening the overall duration of the crop's growth cycle. Insufficient water availability that limits the evapotranspiration also reduces the amount of assimilation and the corresponding yield.

2.2.2 Two-way coupling

In addition to one-way coupling, vegetation-related states and fluxes are passed from WOFOST to PCR-GLOBWB 2 and data exchange between the two models is iterated twice per day. In the two-way coupling, information is exchanged between PCR-GLOBWB 2 and WOFOST as follows (Fig. 1):

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- At the start of the day, WOFOST computes the potential evapotranspiration on the basis of the meteorological variables and the pertinent vegetation states from the previous time step (leaf area index (LAI), rooting depth, and crop height), as well as the actual bare soil evaporation, actual transpiration and the open water evaporation;
- The fluxes are passed to PCR-GLOBWB 2, together with the root depth. The root depth is used to partition the actual transpiration from the single root zone of WOFOST over the two soil layers of PCR-GLOBWB 2, dependent on the root content. For both irrigated and rainfed crops, the actual evapotranspiration from WOFOST is imposed on PCR-GLOBWB 2 and used to update the soil moisture content of the two soil layers in PCR-GLOBWB 2 for the current daily timestep;
- In the case of irrigated crops, the stages of vegetated development are used to compute the amount of irrigation. Potential evaporation is used to calculate the irrigation water demand for paddy crops (not considered here), whereas the irrigation water requirement for non-paddy crops is computed on the basis of the soil moisture status according to the FAO guidelines (Allen et al., 1998). The irrigation water requirement is withdrawn from the available water resources in PCR-GLOBWB 2 and the available irrigation water supply is applied to the crops in addition to any natural precipitation;
- The resulting soil moisture of the two soil layers from PCR-GLOBWB 2 is aggregated to the average value for the root zone of each crop and passed to WOFOST;
- With the soil moisture from PCR-GLOBWB 2, WOFOST computes the actual transpiration and the crop growth and the crop status is updated. The new fluxes and new crop parameters are then passed to PCR-GLOBWB 2 again in the next daily timestep (Fig.1).

In this two-way coupling, the crop phenology from WOFOST determines evapotranspiration and thus the soil hydrology of PCR-GLOBWB 2, particularly during dry spells. Compared to the predefined phenology of PCR-GLOBWB 2, the LAI, rooting depth and evapotranspiration as simulated by WOFOST will lag during dry spells and less water may be lost from PCR-GLOBWB 2. However, the thinner rooting depth will also lead to an earlier drying out of the soil and reduced capillary rise. This subsequently leads to reduced soil moisture (compared to PCR-GLOBWB 2 standalone) which in turn feeds back to a reduced simulated yield in WOFOST, in particular for rainfed crops. For irrigated crops, the extra water supplied will largely offset these feedbacks and result in near-optimum growth.

2.3 Model coupling simulation experiments and parametrization

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Hydrological simulations were conducted with a daily timestep at a 5-arcminute grid resolution, where for each grid cell WOFOST was used to simulate crop growth for irrigated and rainfed maize, soybean, and wheat. To assess the impact of hydrology on crop growth and understand the interactions between hydrology and crop growth, three sets of simulations were carried out for both irrigated and rainfed crops: a) standalone simulations using the WOFOST crop model solely, b) one-way coupled, and c) two-way coupled PCR-GLOBWB 2 - WOFOST simulations. Note that for the standalone simulations with WOFOST under irrigation the potential crop yield is simulated, which is potential yield without water (and nutrient) stress except for temperature effects. When coupled to PCR-GLOBWB 2, water stress can occur even for irrigated crops in case there is not enough water available (in PCR-GLOBWB 2) to fully satisfy the crop water demand. For rainfed crops, growth is influenced by available soil moisture for all simulations and is thus sensitive to water stress and temperature. Green water from natural rainfall is the primary water supply in rainfed analysis, while irrigated crops get water from both green and blue water (from surface water and renewable groundwater) and non-renewable groundwater leading to groundwater depletion.

Daily timestep simulations covered the period from 1979 and 2019, using weather variables (minimum and maximum air temperature, short wave radiation, precipitation, vapour pressure, windspeed, and humidity) from the W5E5 forcing data (Lange et al., 2021) as input to PCR-GLOBWB 2 (Sutanudjaja et al., 2018) and WOFOST. Cropland areas and growing seasons were determined from the MIRCA2000 (Portmann et al., 2010) global monthly irrigated and rainfed crop area dataset. The focus of the coupled framework was to comprehend the impacts and feedback between hydrology and crop growth. Crop parameters, atmospheric CO_2 concentrations, and fertilizer application were obtained from the WOFOST crop parameter dataset for each crop (WOFOST Crop Parameters, 2024). Cultivars in the WOFOST crop parameter datasets were calibrated for each crop against reported agricultural yields from the United States Department of Agriculture (USDA) National Agricultural Statistics Service (USDA, 2024), with the closest matching cultivar selected for final simulations. Detailed information on the cultivar calibration for each crop (i.e. irrigated and rainfed maize, soybean and wheat) is provided in the supplementary information section III.

Comparisons were made between simulations from standalone WOFOST and the one-way and two-way coupled PCR-GLOBWB 2 - WOFOST runs. This comparative analysis involved evaluating the results from different model runs for crop growth against reported crop yields.

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Furthermore, irrigation water withdrawals of coupled model runs are compared against the USGS Water Use Database (USGS, 2023) (section 2.4).

2.4 Model evaluation

We evaluated the three different model configurations by comparing simulated results against reported USDA crop yields of maize, soybean and wheat. Furthermore, we cross-referenced our simulations with irrigation water withdrawal data spanning five years from the USGS Water Use Database. Specifically, we compared data for the years 2005, 2010, and 2015, as the USGS census data is collected at five-yearly intervals.

2.4.1 Crop yields model evaluation

To assess the model's performance, we employ three key metrics: correlation coefficients (r), Normalized Root Mean Square Error (NRMSE) and Normalized Bias (NBIAS). These metrics were selected for their ability to capture the strength, accuracy and systematic errors in the relationship between simulated and observed values.

$$r = \frac{\sum (P_i - \bar{P})(O_i - \bar{O})}{\sqrt{\sum (P_i - \bar{P})^2 \cdot \sum (O_i - \bar{O})^2}} \qquad (1)$$

$$NRMSE = \frac{\sqrt{\frac{1}{n}\sum_{i=1}^{n}(P_i - O_i)^2}}{\bar{O}} \qquad (2)$$

$$NBIAS = \frac{\frac{1}{n}\sum_{i=1}^{n}(P_i - O_i)^2}{\bar{O}} \qquad (3)$$

Where, P_i and O_i are the individual predicted and observed values, respectively and $\bar{P}$ and $\bar{O}$ are the means of the predicted and observed values.

The evaluation was done both temporally for average CONUS yields per year, as well as for multi-year averages per state-per-state to evaluate the model's ability to capture spatial variations in crop yield. This was done for both irrigated and rainfed maize, soybean and wheat.

To further characterize the dataset and evaluate the impact of the degree of coupling on simulated yields, additional statistical analyses were conducted on the 41 years of simulated data at the 5-arcminute grid scale. To this end, the mean and coefficient of variation (CV) were computed for both one-way and two-way datasets for the three crops under irrigated and rainfed conditions. The purpose of this analysis was to examine the central tendency and year-to-year variability of yield simulations and how these are related to the way hydrology and crop growth are coupled.

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2.4.2 Irrigation water use model evaluation

The USGS reported irrigation water use data provides a comprehensive representation of the total irrigation water utilized by all crops for a number of states (USGS, 2023). The irrigated crop area used in this dataset is however not the same as that used in PCR-GLOBWB 2 which is based on MIRCA2000 (Portmann et al., 2010). Thus, directly comparing USGS data with our simulated water withdrawals would result in bias. To ensure a fair comparison between the simulated and reported data, we adjusted the USGS irrigation water use data by multiplying these with the ratio of the irrigated area from MIRCA2000 to the reported total USGS irrigated area. Additionally, our simulated irrigation water withdrawal volumes did not yet account for irrigation efficiency. We intend to implement this in future development. Hence, we introduced an additional correction by dividing the simulated withdrawal data by the irrigation efficiency as is commonly used in PCR-GLOBWB 2 when it is not coupled to a crop model.

After these corrections, the coupled model simulated irrigation water withdrawals were evaluated against actual irrigation data obtained from the USGS database through spatial (multi-year averages per state) and temporal (multi-state totals per year) analysis, providing insights into the model's ability to replicate observed irrigation water use patterns.

This comparison was limited to the years with available reported area data for the simulation period (2005, 2010, 2015) and to the states with reported irrigation water withdrawal volumes for these years (37 states).

3. Results

In this section, we present the key findings obtained from the implementation of the coupled hydrological-crop growth model framework based on WOFOST and PCR-GLOBWB 2. We present our findings sequentially, first delving into observed hydrological impacts on crop growth (one-way coupling) and then exploring how feedback mechanisms between crop growth and hydrology impact the crop growth system (two-way coupling).

3.1 Comparative temporal and spatial analysis of stand-alone, one-way, and two-way coupling for irrigated and rainfed crops

Temporal analysis (Fig. 2) compares the simulated yields with reported yields for irrigated and rainfed maize, soybean, and wheat crops spanning from 1979 to 2019 in the CONUS region. Notably, the reported yields exhibit discernible trends for the CONUS region across the three crops and in both irrigated and rainfed analysis. This temporal evolution is primarily attributed

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to technological advancements, encompassing improved agricultural practices and the introduction of enhanced crop varieties over the study period (Arata et al., 2020).

In contrast, our coupled PCR-GLOBWB 2 – WOFOST model framework simulated yields do not capture such trends, as the modelling approach intentionally omitted to incorporate trends in technology and management practices. For a consistent analysis, we specifically focused on the years when reported yields appear to be more or less stable and in line with our simulated yields. Consequently, the timeframe from 2006 to 2019 was selected for further analysis. Thus, to ensure a meaningful comparison, only the reported yields from 2006-2019 were used for evaluating the accuracy and reliability to ensure a fair and meaningful comparison of simulated yields.

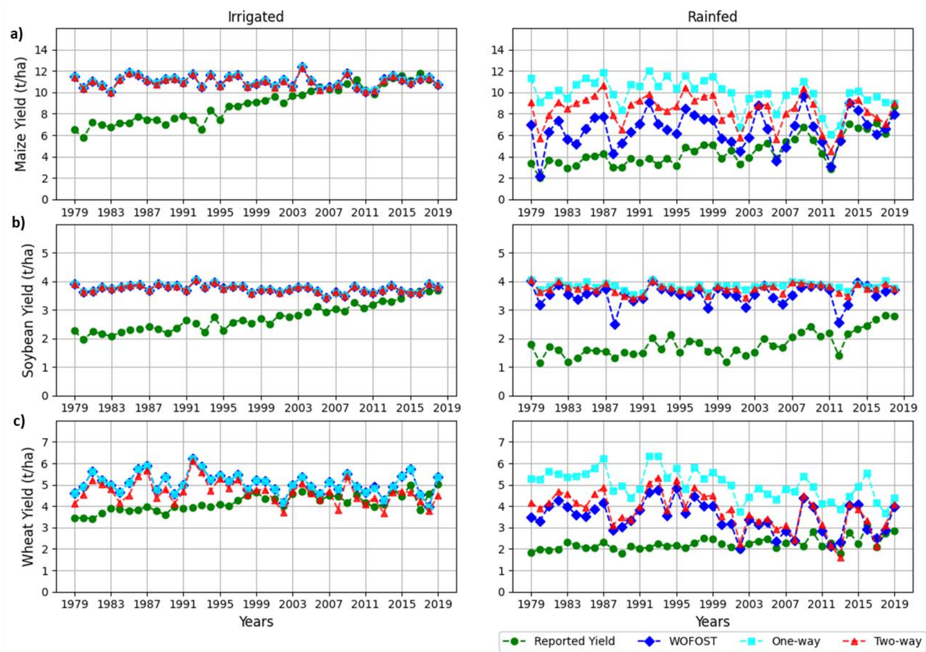

Figure 2: Temporal analysis of irrigated and rainfed crops of a) maize, b) soybean and c) wheat for the years 1979 to 2019 of a CONUS region

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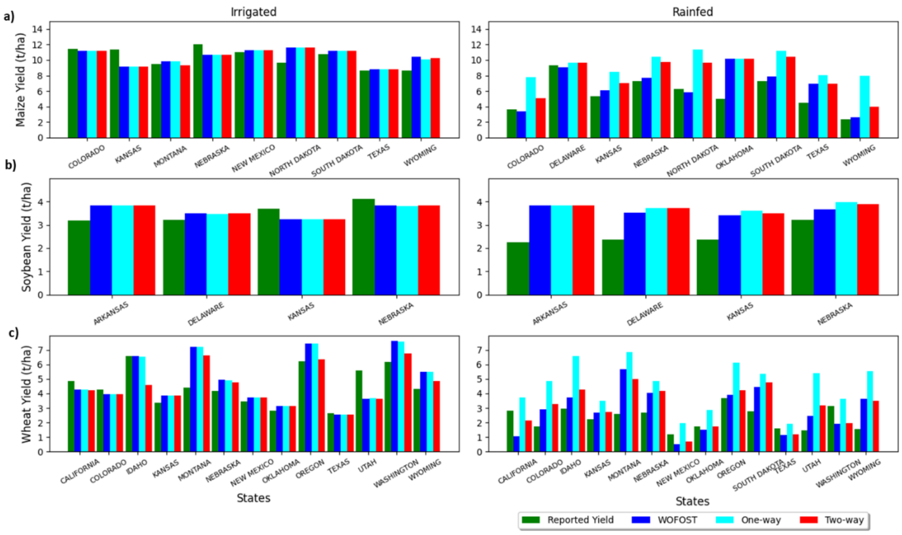

Figure 3: Spatial (i.e. state level) analysis of irrigated and rainfed crops of a) maize, b) soybean and c) wheat for the years 2006 to 2019 for the CONUS region.

Figures 2 and 3 show the outcomes of comparing simulated irrigated and rainfed analyses yields for maize, soybean, and wheat with reported yields. For the irrigated crops, the obtained yields by standalone WOFOST represent the potential productivity for the three crops. Notably, one-way, and two-way model runs for irrigated crops yielded nearly identical results to the standalone runs, indicating that there is generally enough irrigation water to completely satisfy crop water demands. Although not shown here, we note that this is at the expense of non-renewable groundwater use in states overlying the Southern Great Plains aquifer system. Conversely, for rainfed crops, the stand-alone and two-way simulations produced comparable results, while the one-way coupling approach exhibited an overestimation of yields relative to stand-alone and two-way simulations particularly for wheat and to a lesser degree for maize. This discrepancy arises from the fact that in one-way coupling soil moisture calculations in PCR-GLOBWB 2 under drought conditions assume a full rooting depth development (the phenology is fixed) which could, as described before, lead to an over-estimation of soil moisture that is then passed to WOFOST, eventually leading to an overestimation of yield. In contrast, the two-way coupling approach feeds back information about the lagging behind of crop development to PCR-GLOBWB 2, which results in more realistic soil moisture and crop yield simulations by the two-way coupling.

The analysis of temporal variations in simulated irrigated and rainfed maize crop yields shows distinct year-to-year fluctuations. Rainfed maize, in particular, exhibits a discernible pattern

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with certain years marked by notable peaks in yields, contrasting with others that experienced comparatively lower production, revealing sensitivity to varying environmental conditions. These variations are also observed in reported maize yields. Similar year-to-year patterns are found for simulated irrigated and rainfed wheat yields, but not so in observed yields. Apparently, sensitivity to water and/or temperature variability in WOFOST is larger than observed. Also, a significant discrepancy emerges in irrigated and rainfed soybean yields, where simulated yields surpass the reported values, particularly in rainfed conditions.

In the spatial analysis, simulated irrigated maize yields from stand-alone (WOFOST), one-way, and two-way coupling align almost identical with reported irrigated maize yields. Conversely, in rainfed maize analysis, stand-alone and two-way simulations outperform reported yields in states such as Colorado, Kansas, North Dakota, and Wyoming, while one-way coupling exhibits an overestimation of yields compared to stand-alone (WOFOST) and two-way coupling.

For soybeans, the spatial analysis reveals identical yields among stand-alone (WOFOST), one-way, and two-way simulations for both irrigated and rainfed crops. For irrigated crops, simulated yields were overestimated in states like Arkansas and Delaware and underestimated in Kansas and Nebraska compared to reported values. For irrigated and rainfed wheat, simulated yields of the two-way coupling outperform stand-alone WOFOST and one-way coupling, particularly in states like Idaho, Montana, Oregon, and Wyoming. The one-way coupling, lacking feedback from the crop growth model to the hydrological model, leads to an overestimation of rainfed yields across all states compared to stand-alone WOFOST and two-way coupling. This underscores the importance of incorporating two-way interactions and feedback mechanisms for more accurate yield simulation results.

3.2 Evaluation statistics

Table 1 presents model performance metrics (correlation, normalized RMSE and normalized bias), evaluating simulations for the three model setups (i.e. standalone WOFOST, one-way, two-way coupling) for irrigated and rainfed maize, soybean, and wheat.

For irrigated crops, simulation approaches exhibit positive correlations. Specifically, for maize, the correlation coefficients are high (0.63), moderate for soybean and rather low for wheat. The normalized root mean square errors (RMSE) remain consistently low, with values ranging from 0.13 to 0.18 across three crops, indicating a reasonable fit of the simulated values to the observed data. Moreover, normalized biases are also low, ranging from 0.01 to 0.20. The two-

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way coupling demonstrates overall slightly lower biases compared to stand-alone and one-way simulations, particularly for wheat.

Table 1: Model performance metrics (i.e. correlation, normalized RMSE and normalized bias) for simulated irrigated and rainfed maize, soybean, and wheat.

S.No	Metrics	Maize			Soybean			Wheat		
Irrigated crops		Stand alone	One-way	Two-way	Stand alone	One-way	Two-way	Stand alone	One-way	Two-way
1	Correlation	0.63	0.63	0.63	0.46	0.46	0.45	0.22	0.22	0.24
2	Normalized RMSE	0.13	0.13	0.13	0.06	0.06	0.06	0.18	0.18	0.18
3	Normalized Bias	0.20	0.20	0.20	0.01	0.01	0.01	0.12	0.12	0.06
Rainfed crops										
1	Correlation	0.77	0.65	0.77	0.57	0.22	0.33	0.44	0.51	0.55
2	Normalized RMSE	0.22	0.50	0.50	0.42	0.57	0.57	0.37	0.66	0.66
3	Normalized Bias	0.31	1.65	0.84	0.42	0.78	0.63	0.28	0.91	0.32

For rainfed crops, the correlation coefficients vary, with two-way coupling displaying the highest correlations. Higher correlation coefficients are obtained for maize (0.65-0.77) compared to soybean (0.22-0.57) and wheat (0.44-0.55). Normalized RMSE values are generally higher in rainfed conditions compared to irrigated, ranging from 0.22 to 0.66. Normalized biases show variations across simulation approaches and crops, ranging from 0.28 to 1.65. Specifically, one-way coupling exhibits higher biases in rainfed maize, soybean and wheat compared to stand-alone and two-way simulations.

Overall, the validation results affirm the overall effectiveness of the simulation approaches in accurately representing observed irrigated and rainfed crop yields, with stand-alone and two-way coupling slightly outperforming one-way simulations.

3.3 Relevant feedbacks revealed by two-way coupling between hydrology and crop growth

We further investigated the impact of the developed model coupling by looking at its impact on simulated crop yield in terms of the CONUS-wide 5-arcminute spatial variation and multi-year variability. To evaluate the impact of coupling dynamics, we assessed key indicators, including mean crop yields, the coefficient of variation (CV) of crop yields expressing interannual variability, and the relative difference in mean and CV between two-way and one-way couplings.

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Spatial patterns of the 1979-2019 mean simulated crop yields of maize, soybean and wheat are shown under irrigated (Fig. 4) and rainfed (Fig. 5) conditions across the CONUS region. For irrigated crops (Fig. 4), the regions show similar yields for one-way and two-way coupled simulations, which is expected since soil moisture is kept at optimal conditions so that feedbacks from WOFOST to PCR-GLOBWB 2 are inconsequential. For rainfed conditions (Fig. 5), where water availability relies on green water, the yields are comparatively lower than in irrigated conditions. Also, differences between one-way and two-way coupled simulations emerge in the western part of the CONUS. Notably, one-way coupling tends to simulate higher yields for maize and wheat compared to two-way coupling. This discrepancy arises from the transmission of soil moisture from the hydrological to the crop growth model in one-way coupling, without receiving feedback from crop development to the hydrological model. As stated before, this may overestimate soil moisture availability under drier conditions subsequently leading to a likely overestimation of simulated crop yield by the one-way coupling. Clearly, this feedback is more important in the western part of CONUS, which is likely related to larger interannual climate variability (with more dry conditions) compared to the eastern part (see the section hereafter). The larger differences in mean yields for rainfed crops, particularly in the western CONUS, that occur between one-way and two-way coupled simulations are further illustrated by looking at the relative differences between the two coupling methods (see Supplementary Information IV; Fig. S5).

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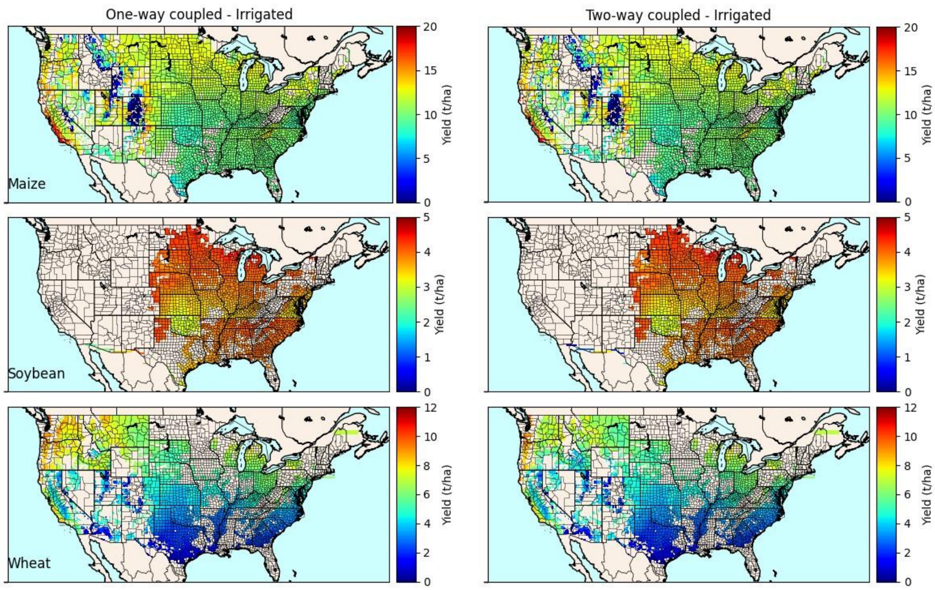

Figure 4: Mean irrigated crop yields for maize, soybean, and wheat within CONUS as obtained from one-way and two-way coupled simulations for 1979-2019.

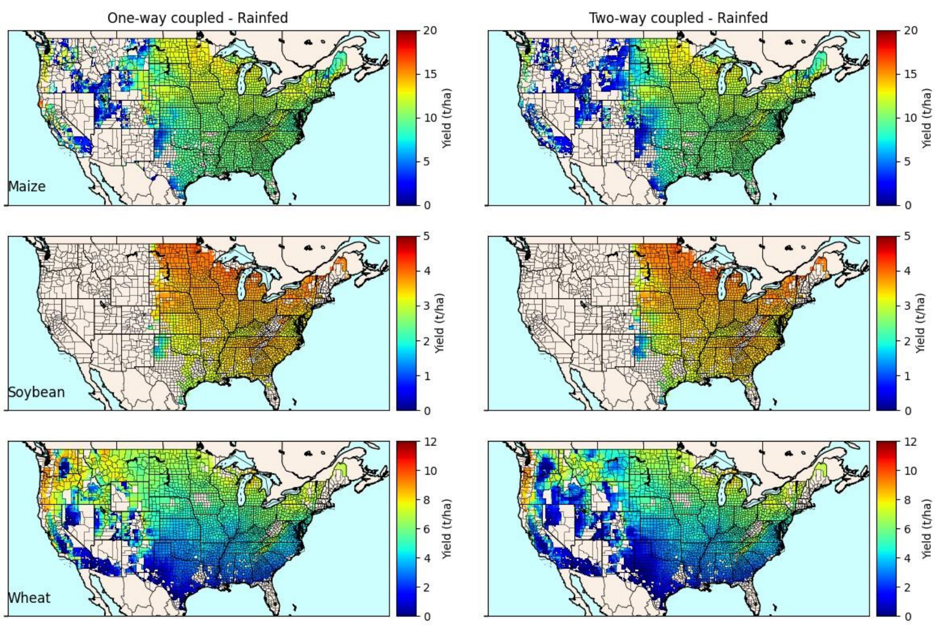

Figure 5: Mean rainfed crop yields for maize, soybean, and wheat within CONUS as obtained from one-way and two-way coupled simulations for 1979-2019.

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Spatial patterns of the coefficient of variation (CV) (in % of the mean) across CONUS for maize, soybean and wheat are shown under irrigated (Fig. 6) and rainfed conditions (Fig. 7) comparing the simulations of the one-way and two-way coupling. High CV values entail a larger inter-annual variability in crop yield.

In the eastern part of CONUS, the CV values both in irrigated and rainfed conditions are notably lower, suggesting a more stable and consistent pattern of crop growth in these regions. Conversely, in the mid-western and western CONUS, inter-annual variability is higher, owing to larger inter-annual climate variability in these parts. For irrigated crops, a larger CV is mostly apparent for maize and wheat. For a small number of instances, this could be caused by insufficient irrigation water availability during very dry and hot years, but most likely this is a temperature signal. Also, we note that in these parts of CONUS, some pixels have very low to minimal cropping areas, resulting in more pronounced fluctuations in yields. As can also be seen from Supplementary Information IV Fig. S6, the differences between one-way and two-way coupled runs are generally small, except for some northwestern states.

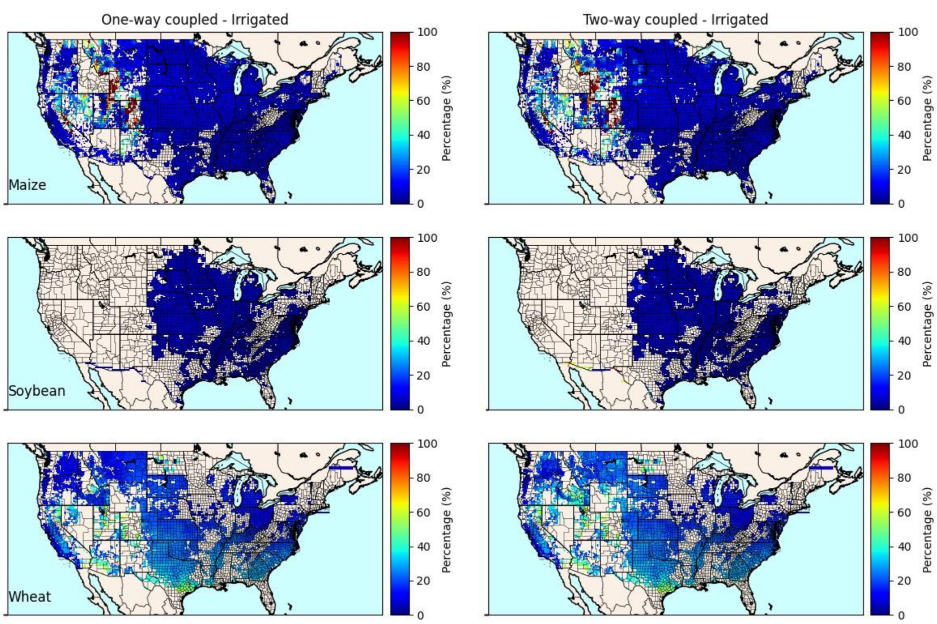

Figure 6: Coefficient of Variation (CV) over 1979-2019 of irrigated crop yields for maize, soybean, and wheat within CONUS as obtained under one-way and two-way coupling

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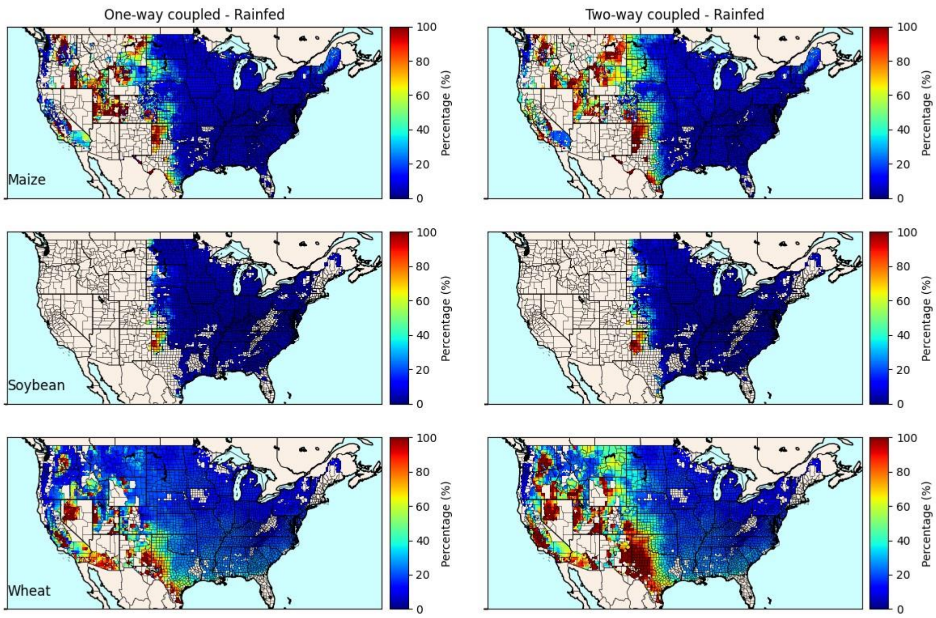

Figure 7: Coefficient of Variation (CV) over 1979-2019 of rainfed crop yields for maize, soybean, and wheat within CONUS as obtained under one-way and two-way coupling

Rainfed crops show larger values of CV, especially in the western part of CONUS, reflecting the larger sensitivity of rainfed agriculture to inter-annual climate variability (Fig. 7). It is also clear that the simulated inter-annual variability of simulated crop yield is larger for two-way than for one-way coupling, reflecting the importance of including crop phenology, in particular variation in rooting depth, when simulating available soil moisture. We also refer to Supplementary Information IV Fig. S6 for relative differences between the two model coupling approaches. This larger inter-annual variability also partly explains the lower mean yields for rainfed crops and two-way coupling as was shown in Fig 5.

3.4 Irrigation water use

The scatter plot (Fig. 8) shows the relationship between reported USGS (after correction for area and irrigation efficiency – see 2.4) and simulated irrigation water withdrawals under one-way and two-way coupling. The plot shows that the simulated irrigation water withdrawals are correct in order of magnitude when compared to reported data across different states. The temporal variations (Fig. 9) illustrate that year-to-year changes in total irrigation water withdrawal over time are small for both one-way and two-way coupling and the reported totals.

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Figures 8 and 9 show that irrigation water withdrawal is underestimated in total and for most states. The underestimation of irrigation water use by PCR-GLOBWB 2 was previously noted by Ruess et al., (2023). This underestimation was partly accounted for when using more detailed crop cover data, irrigation efficacies and meteorological forcing than currently used in the global version of PCR-GLOBWB 2.

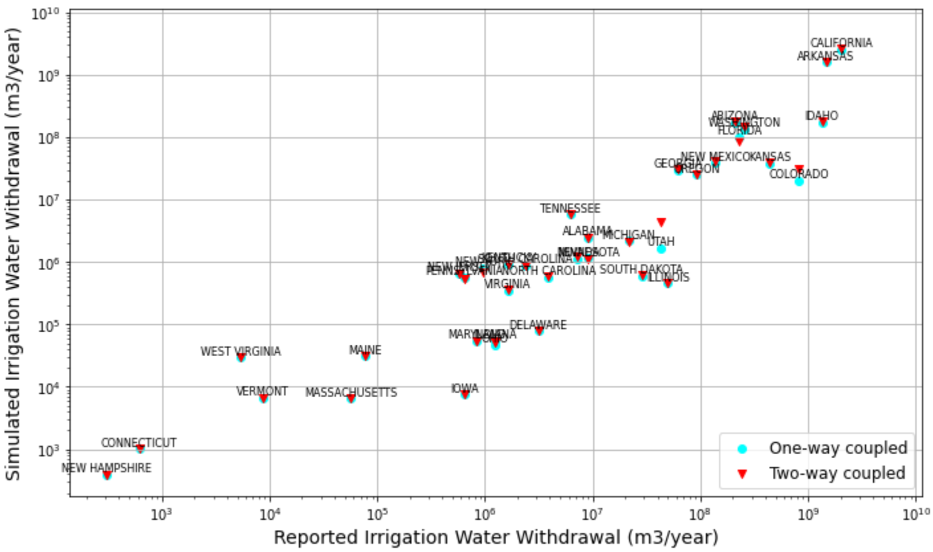

Figure 8: Spatial variation of one-way and two-way irrigation water withdrawal compared with USGS water withdrawal data across the CONUS region with a logarithmic scale

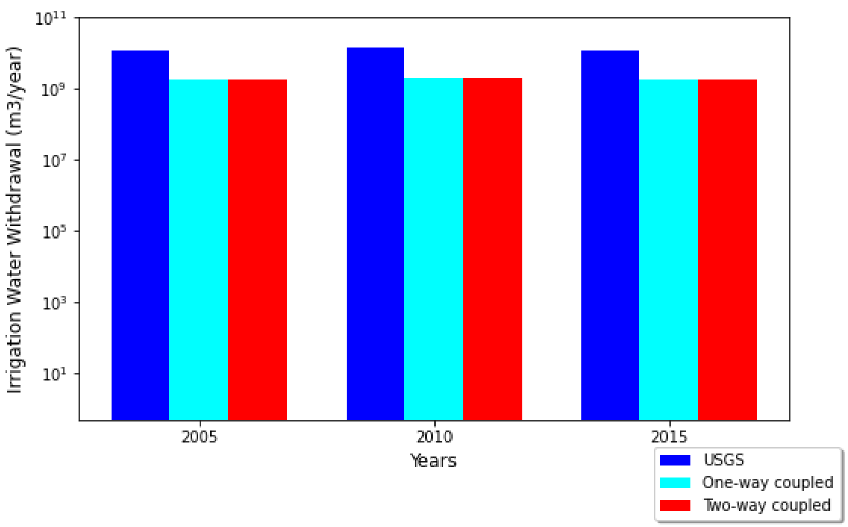

Figure 9: Temporal variation of one-way and two-way irrigation water withdrawal compared with USGS water withdrawal data of 5-year intervals across the CONUS region with a logarithmic scale

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4 Discussion and Conclusion

In this study, we developed a coupled hydrology-crop model framework to investigate the intricate feedbacks between water availability and crop growth within the CONUS region focusing on maize, soybean and wheat. This discussion delves into the implications of the findings, emphasizing their significance and addressing both methodological considerations and inherent uncertainties.

The spatiotemporal analysis of hydrological impacts on crop growth reveals distinctive patterns for both irrigated and rainfed conditions. Notably, the improved performance of the two-way coupling in capturing more realistic yield outcomes for rainfed conditions highlights the importance of incorporating the full feedback loop between hydrology and crop growth. The discrepancy in one-way coupling results, leading to overestimation in simulated compared to reported yields, underscores the importance of feeding back the actual crop phenology to the hydrological model in coupled hydrology-crop growth modelling.

Our studies adds to previous work by Droppers et al., (2021), which investigated worldwide water constraints and sustainable irrigation by coupling the Variable Infiltration Capacity (VIC) hydrological model with WOFOST and Zhang et al. (2021) who focused on refining the coupled VIC hydrological model with a crop growth model EPIC by incorporating the evapotranspiration module at a regional scale. In comparison, our research extends the analysis to a finer spatial scale and places a stronger emphasis on the comprehensive integration of feedback loops between hydrology and crop growth. Particularly, we demonstrate the importance of two-way coupling in capturing realistic yield outcomes, which is particularly evident for rainfed crops. This is mainly because the two-way coupled system addresses the influence of crop status on evapotranspiration and rooting depth, thereby impacting soil moisture content, which in turn feed backs on crop growth. The two-way coupling approach provides a more realistic depiction of water availability for crops, which results in larger inter-annual variability and lower mean crop yields when inter-annual climate variability is significant. Including this two-way interaction is particularly important under drier conditions or if the coupled framework is used to assess reduced surface water availability under climate change or the impact of environmental constraints on groundwater and surface water use. The significance of implementing a two-way coupling between hydrology and crop growth is also evident when calculating high-resolution long-term mean crop yields and inter-annual variability of yield, as measured by the coefficient of variation (CV) of simulated yield. In

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irrigated conditions, both one-way and two-way coupling yield similar results, demonstrating the stability in water availability.

Validation results affirm the reliability of the coupled PCR-GLOBWB 2 – WOFOST model framework, demonstrating close agreement with observed data through overall strong positive correlations, low normalized RMSE, and minimal bias. Here, the difference in performance between one-way and two-way coupling is small. In rainfed conditions, where variability is inherent, the better performance of two-way coupling emphasizes the added value of dynamic feedback mechanisms for more accurate simulation results. Even though the stand-alone WOFOST performed similarly to the two-way coupled model framework, the latter is still beneficial for comprehensively understanding the joint impacts on both crop growth and irrigation water use, particularly in situations of limited water availability.

While the results of this study offer valuable insights into the coupled hydrology-crop model framework, it is essential to recognize and address the uncertainties associated with the structure and parametrization, as well as inherent limitations in the research. A significant limitation is that the study does not account for potential advancements in agricultural technology and evolving farming practices, which could impact crop yields (section 3.1; Fig. 2). The ignorance of technological innovations may contribute to discrepancies between simulated and actual yields.

Furthermore, uncertainties linked to input datasets (Porwollik et al., 2017; Roux et al., 2014) such as crop calendars, cultivars and land-use changes introduce potential limitations and implications for the study results. Accurate representations of crop growth dynamics hinge on accurate crop calendar definitions (Wang et al., 2022), encompassing planting, maturation, and harvesting periods. Variations in these timelines due to climate change or evolving agricultural practices potentially introduce uncertainties in yield predictions. Additionally, the assumption of static cultivars neglects potential shifts in agricultural practices or the introduction of new varieties, influencing crop growth responses to environmental stressors over time. Land-use changes further contribute to uncertainties (Prestele et al., 2016; Eckhardt et al., 2003; Dendoncker et al., 2008) as dynamic shifts in agricultural practices alter water demand, evapotranspiration patterns, and overall hydrological dynamics. Ignoring these potential shifts limits the model's ability to capture the complex interactions between water and crop systems, and this should be considered in future development steps.

Hence, future work should also consider representing the dynamic nature of crop areas, including both irrigated and rainfed crop harvest areas, as well as the total crop area. The assumption of constant areas, as made in prior studies (Müller et al., 2017; Ai and Hanasaki, 2023; Jägermeyr et al., 2021) was based on data availability constraints, but acknowledging the potential variability in these factors over time. Addressing this aspect is crucial for enhancing the accuracy of yield calculations and, consequently, advancing the overall understanding of hydrology-crop growth interactions. The integration of such variability into modelling frameworks is not only essential for improving the accuracy of assessments but also for contributing to an enhanced understanding of the broader water-food nexus.

In conclusion, the development and application of the two-way coupled hydrology-crop growth model framework presented in this study represents a significant advancement in our ability to understand the cascading mechanisms and feedbacks between water and crop systems. This versatile framework not only enhances our understanding of the interplay between hydrology and crop growth but, through the sectoral water use modules of PCR-GLOBWB 2, has the necessary components to evaluate large-scale water use management strategies, and simulate the large-scale impacts of informed decision-making under change, particularly when dealing with hydroclimatic extremes.

Author contribution

SC designed the study, performed the analyses, validation and visualization of the results under the supervision of LPHvB, MTHvV and MFPB. SC developed the coupled framework in close collaboration with LPHvB. JA contributed to the conceptualization of software. SC wrote the original draft manuscript and all co-authors reviewed and edited the manuscript.

Code and data availability

The developed coupled PCR-GLOBWB 2-WOFOST model framework is available at https://zenodo.org/doi/10.5281/zenodo.10681452. The datasets used in the coupled model framework are available at https://opendap.4tu.nl/thredds/catalog/data2/pcrglobwb/version_2019_11_beta/pcrglobwb2_input/catalog.html.

Competing interests

The contact author has declared that none of the authors has any competing interests.

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