Relevance of feedbacks between water availability and crop systems using a coupled hydrological – 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

38 with hydrological models, a two-way coupling is needed to capture the impact of interannual

39 climate variability on food production.

1 Introduction

42 Global trends in population and economic growth are expected to increase the demand for

43 water, food, and energy, threatening the sustainable and equitable use of natural resources

44 (Sophocleous, 2004; Tompkins and Adger, 2004). Water as a resource plays a crucial role in

45 crop growth, cooling of thermoelectric plants, hydropower generation, and covering domestic

46 and industrial demand. Water, therefore, is an essential resource at the core of the Water-

47 Energy-Food-Ecosystem (WEFE) nexus. Currently, 70% of total global freshwater

48 withdrawals are accounted for by agriculture, making it the largest water user among all sectors

49 (Dubois, 2011). The Food and Agriculture Organization (FAO) of the United Nations estimated

50 that the demand for water and food resources will likely increase by 50% by 2050 compared

51 to 2015 (IRENA, 2015; Corona-López et al., 2021). The increasing demand for water and food

52 will likely have negative impacts on the environment and will inhibit socio-economic

53 development if a gap opens between growing water demand and water availability.

54 The critical interplay between hydrology and crop growth becomes evident during

55 hydroclimatic extremes (e.g. droughts, heatwaves), as rising demands coincide with potential

56 declines in both water resources and food production (crop yield) (Jackson et al., 2021). In

57 addressing the complexities associated with these challenges, studies by Jägermeyr et al.

58 (2017), utilizing a dynamic vegetation model (LPJmL), evaluated achievable irrigated crop

59 production under sustainable water management. Their findings revealed that 41% of global

60 water use currently compromises environmental flow requirements crucial for river

61 ecosystems, potentially leading to losses in irrigated croplands. Concurrently, research by

62 Vörösmarty et al. (2000) and Leclère et al., (2014) projects the impacts of climate change on

63 global agricultural systems, foreseeing an increase in irrigated areas in the future, underscoring

64 the necessity for significant investments in irrigation, energy, and water resource management.

65 These findings emphasize the urgent need for improved modelling approaches to assess the

66 complex interaction between water availability, climate change and crop yields.

67 BiophysicalTo address these challenges, biophysical process-based models, as highlighted by

68 have been widely used to study the interactions between hydrology and crop growth (Siad et

69 al., (2019); and Zhang et al., (2021), are instrumental in understanding the intricate relationship

70 ~~between hydrology and crop growth, particularly in response to changing hydroclimatic~~

71 ~~conditions. Considering factors like irrigation water use and soil-groundwater dynamics, these~~

72 ~~.~~ These models ~~explore~~provide valuable insights into how meteorological events influence

73 water availability for crops, as well as ~~the impacts of diminished~~how changes in crop growth

74 and ~~premature~~ senescence ~~on hydrology through effects on root water uptake and~~affect

75 hydrological fluxes such as evapotranspiration~~. This understanding becomes crucial when~~

76 ~~assessed at the regional to global scale, where local deficits can have cascading consequences~~

77 ~~for both water and food security.~~

78 ~~In the context of studying the impact of climate change and variability on crop yields, aside~~

79 ~~from biophysical models, numerous crop models have been employed.~~ and root water uptake.

80 However, ~~these~~existing stand-alone crop models and hydrological models often simplify these

81 processes. For instance, crop models usually incorporate a simplified soil-water balance

82 (Zhang et al., 2021) that overlooks local hydrological processes and often do not account for

83 water use for irrigation and non-agricultural sectors. Conversely, most hydrological models

84 simplify or neglect the effects of land cover, phenology and vegetation changes on hydrological

85 fluxes and the state of available water resources (Tsarouchi et al., 2014). These simplifications

86 arise due to computational expediency, disparities in process scales between hydrology at the

87 river basin level and crop yield at the field level, incomplete understanding of the other domain

88 by model developers, or because of epistemological uncertainty (Siad et al. 2019; McMillan et

89 al., 2018; Shafiei et al. 2014). Recognizing the strengths of both crop models and ~~global~~

90 hydrological models, a coupling allows for the exploration of dynamic crop growth's influence

91 on hydrology and water use ~~and~~. Additionally, a model coupling allows the incorporation of

92 ~~accurate~~ spatio-temporal variations in hydrological fluxes, including water use, in estimates of

93 crop yield. This understanding becomes crucial when assessed at the regional to global scale,

94 where local deficits can have cascading consequences for both water and food security at the

95 basin scale.

96 The rationale for coupling hydrological and crop growth models is twofold. First, coupling

97 these models allows for the possibility to assess the impact of limited irrigation water

98 availability on crop yield. Second, it enables a detailed analysis of how changes in crop type

99 and growth stages influence groundwater and surface water availability, particularly through

100 processes such as evapotranspiration and root water uptake. By combining a hydrological

101 model with a crop growth model, this study aims to enhance our understanding of hydrological

and crop growth interactions and their implications for agricultural productivity and water resource management on the continental scale.

Previous studies have attempted to couple hydrological and crop models. 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 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~~this study aims to quantify the two-way

interactions between crop growth and hydrology, hypothesizing that coupling a crop growth model with a hydrological model will improve both crop yield and hydrological predictions by incorporating dynamic feedbacks between water availability and crop processes. Specifically, we hypothesize that: (1) a more realistic representation of soil moisture dynamics and water availability will lead to better estimates of water stress and yield; and that (2) directly integrating crop growth information into hydrological models will enhance the accuracy of predictions regarding irrigation needs and water resource allocation. To test these hypotheses, we compare three modeling approaches: a stand-alone crop model, a one-way coupled model (where hydrological conditions influence crop growth but not vice versa), and a two-way coupled model (where interactions between hydrology and crop growth are fully represented). By evaluating these different approaches, we aim to determine whether dynamic hydrological-crop growth feedbacks improve the performance of crop yield and irrigation water use simulations.

Although this study has a 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 investigate the intricate feedback between water availability and crop growth, focusing on three key scientific objectives: 1) assessing the impacts of irrigation and hydrology on crop growth; 2) investigating the feedbacks of crop growth on the hydrological system when accounting for interannual variability; and 3) evaluating 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

165 between hydrology and crop growth, thereby addressing the current research gap in a more
166 comprehensive manner.

167 The rationale behind coupling the hydrological and crop growth models lies in the need to
168 accurately capture the dynamic interactions between these systems, ensuring that both the water
169 availability and crop growth are represented with a sufficient level of sophistication in the
170 simulations to understand crop water interactions. The coupling allows for the exchange of
171 critical variables such as soil moisture, evapotranspiration, and crop water uptake, which are
172 essential for understanding and predicting the impacts of environmental changes on agricultural
173 productivity and water resources. The justification for this coupling, including its expected
174 benefits and the technical approach, is detailed in section 2.2.

175 We hypothesize that the feedback between hydrology and crop growth is significant and
176 complex. Changes in soil moisture and water availability are expected to directly influence
177 crop water uptake, growth rates, and yield outcomes. Conversely, crop processes such as
178 evapotranspiration and root water uptake are likely to impact soil moisture levels, groundwater
179 recharge, and surface water flows, thereby altering water resources. Furthermore, we anticipate
180 that the integration of real-time crop data into hydrological models will enhance the accuracy
181 of predictions regarding water stress, irrigation needs, and crop productivity.

182 To address this To test the hypotheses coined above, the PCR-GLOBWB 2 hydrological model
183 (Sutanudjaja et al., 2018) is coupled to the WOFOST crop model (de Wit et al., 2019) at a daily
184 timestep and at a 5-arc minute (~10 km) spatial resolution applied to CONUS (section 2.1). In
185 examining the interaction between hydrology and crop growth, we consider both one-way and
186 two-way interactions. First, a one-way coupling is established to evaluate the effect of the
187 simulated water availability of PCR-GLOBWB 2 for rainfed and irrigated crop growth in
188 WOFOST (section 2.1; section 2.3.1). In addition, a two-way coupling is established in which,
189 additional to passing water availability from PCR-GLOBWB 2 to WOFOST, the crop
190 phenology of WOFOST in terms of actual evapotranspiration, leaf area index and rooting depth
191 is fed back into PCR-GLOBWB 2 (section 2.1, 2.3.2;).). The justification for this coupling
192 approach, along with technical implementation details, is elaborated upon in section 2.2.

193 Furthermore, our Our framework was tested by comparing individual WOFOST and coupled
194 one-way and two-way model runs to evaluate the impact of feedbacks on crop yield and
195 irrigation water use (section 2.4). The results of these simulations are compared with and
196 evaluated against reported yield statistics and reported annual irrigation withdrawals to assess

197 their validity (section 2.5; section 3). In the end, we elaborate on the uncertainties, strengths,

198 and usability of our coupled model framework for studying the water-food nexus under global

199 change (section 4).

200

201 **2   Methods**

202 A newly coupled hydrological-crop model framework (Fig. 1) is developed to include the

203 feedback between crop growth and hydrology. Here, we chose WOFOST as the crop growth

204 model because of its detailed crop phenology and development and PCR-GLOBWB 2 as the

205 hydrological model because of its detailed hydrological process simulation and large-scale

206 applicability. This framework includes both a one-way and two-way coupling between the

207 PCR-GLOBWB 2 global hydrological and water resources model (Sutanudjaja et al., 2018)

208 and the WOFOST crop growth model (de Wit et al., 2019). The coupled framework was then

209 used to quantify the impacts of included feedbacks between hydrology and crop growth on a

210 daily timestep and 5 arcminutes resolution for CONUS.

211 The following (sub)sections provide a description of the PCR-GLOBWB 2 and WOFOST

212 models and modules used (2.1), justification of coupling (2.2), the model coupling setup (2.3),

213 model coupling simulation experiments and parametrization (2.3), validation of crop yield and

214 of irrigation water use (2.4).

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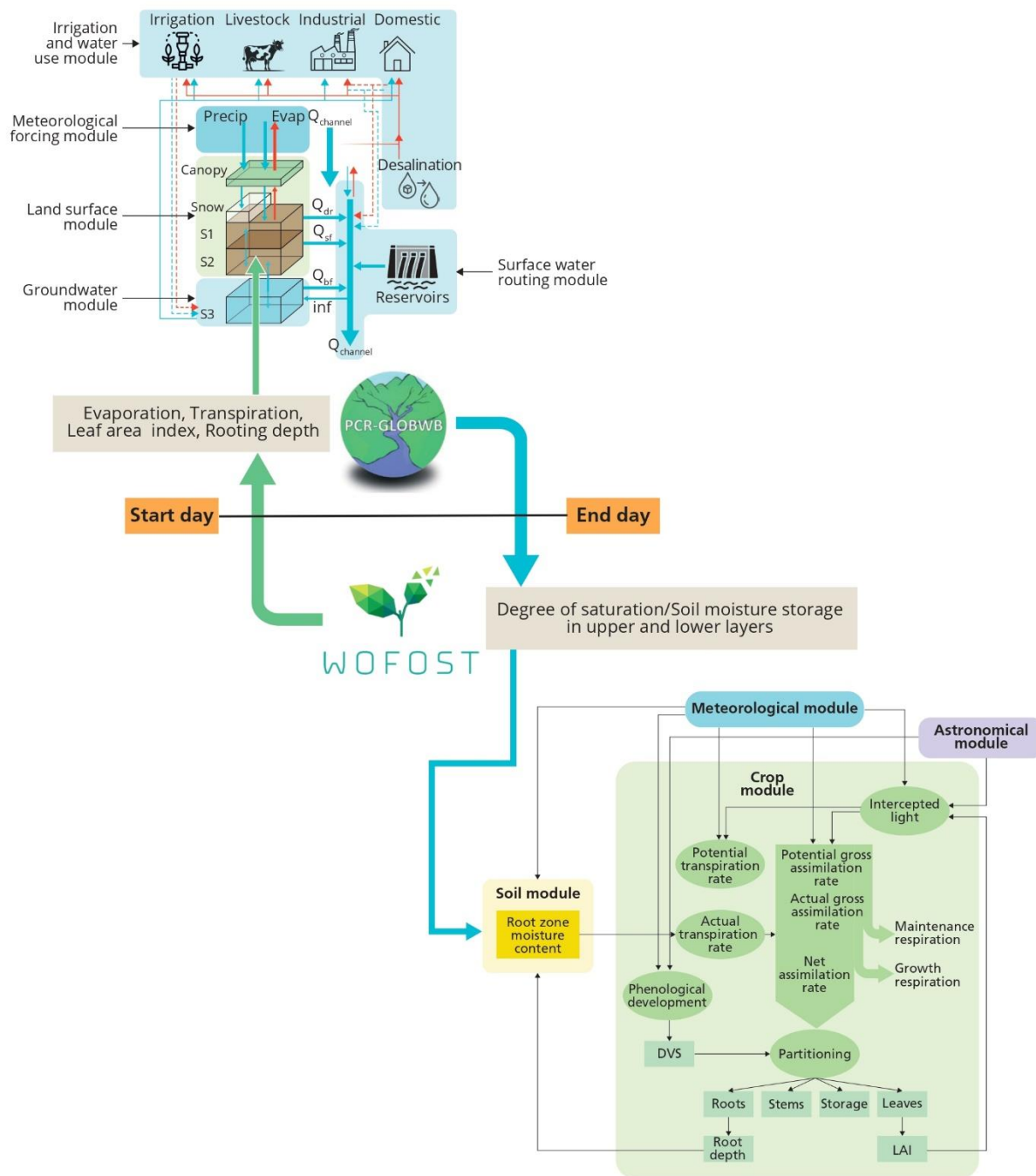
Figure 1: The coupled model framework of the PCR-GLOBWB 2 hydrological and water resource model and the WOFOST crop growth model along with their model structures. The blue arrow represents the one-way coupling from PCR-GLOBWB 2 to WOFOST and the variables that are exchanged; the green arrow is added 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.

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224

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2.1. Model ~~description~~descriptions

PCR-GLOBWB 2

The PCRaster Global Water Balance (PCR-GLOBWB 2) model (Sutanudjaja et al., 2018), developed at Utrecht University, is a global hydrological and water resource model that operates on a latitude-longitude grid. This model simulates the terrestrial hydrological cycle with daily resolution, incorporating anthropogenic impacts like man-made reservoirs, sectoral water demands, withdrawals, consumptive use, and return flows. PCR-GLOBWB 2 is applied and tested across local to global scales.

PCR-GLOBWB 2 utilizes time-explicit schemes for all dynamic processes, running on daily time steps for hydrology and water use, and sub-daily steps for hydrodynamic river routing. It simulates moisture storage in two upper soil layers and manages water exchange among the soil, atmosphere, and groundwater. Atmospheric interactions include precipitation, evaporation, transpiration, and snow processes. The model considers sub-grid variability in land use, soils, and topography, influencing run-off, interflow, groundwater recharge, and capillary rise. Run-off is routed through river networks using methods ranging from simple accumulation to kinematic wave routing, supporting floodplain inundation and surface water temperature simulation.

The model includes a reservoir operation scheme for over 6000 human-made reservoirs from the GRanD database, integrated according to their construction year. Human water use is comprehensively modeled, estimating sectoral water demands and converting them into withdrawals from groundwater, surface water, and desalination sources, while accounting for resource availability and groundwater pumping capacity. Consumptive use and return flows are calculated for each sector.

PCR-GLOBWB 2's flexible structure encompasses five main hydrological modules: meteorological forcing, land surface, groundwater, surface water, irrigation, and water use. The meteorological module uses gridded temperature and precipitation data. Reference potential evaporation is calculated using Hamon's method and employed in the land surface module to determine crop-specific potential evaporation. The groundwater and surface water modules handle fluxes and stores for groundwater and surface water, respectively. The irrigation and water use module simulates water demand, withdrawals, consumption, and return flows, sourcing water from surface water (rivers and reservoirs), groundwater (both renewable and

non-renewable), and desalinated water, depending on availability. Detailed descriptions of each module are 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 (Droppers et al. 2021).

The WOFOST crop model comprises of four modules: meteorological, crop, astronomical 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.

Temperature effects on crop development within WOFOST are modeled using temperature sums, which accumulate daily temperatures above a specified threshold. These sums influence germination and phenological stages, thereby affecting CO2 assimilation. Additionally, the model accounts for the direct and indirect effects of suboptimal daytime temperatures on crop growth and development, which are critical to overall plant performance. Daily photosynthesis in the crop growth model is simulated by considering absorbed radiation and water stress. After accounting for the assimilates used in maintenance respiration, the remaining resources are allocated among the plant's leaves, stems, roots, and storage organs. A key internal driver of this process is the leaf area index (LAI), which results from leaf area dynamics governed by photosynthesis, biomass allocation, leaf age, and developmental stage. LAI, in turn, influences the daily rates of photosynthesis.

WOFOST has been finely tuned to account for diverse climate and soil conditions, particularly for commonly studied crops such as maize, soybean, and wheat, thereby, reducing the need for further recalibration. This pre-tuning ensures that simulations reliably capture the growth and yield responses of these crops under varying environmental conditions. For more detailed information on the fine-tuning of crop variables, see (de Wit and& Boogaard, 2021).

289   WOFOST employs a classic water balance approach designed for freely draining soils where
290   groundwater is too deep to affect soil moisture content in the rooting zone. This approach
291   divides the soil profile into two compartments: the rooted zone and the lower zone extending
292   from the actual rooting depth to the maximum rooting depth. The subsoil below this maximum
293   rooting depth is not considered. As roots extend deeper towards the maximum rooting depth,
294   the lower zone gradually merges with the rooted zone. This approach is suitable for regional
295   applications with limited soil property information. Soil moisture in the root zone serves as a
296   primary link between the WOFOST model and the underlying soil module. For a detailed
297   description of the WOFOST crop growth model, we refer to de Wit and& Boogaard, (2021)
298   and Supit et al., (1994).

299   **2.2. Justification of model coupling**

300   The integration of the hydrological model PCR-GLOBWB 2 (Sutanudjaja et al., 2018) with
301   the crop growth model WOFOST (Supit et al., 1994) is crucial for accurately simulating the
302   complex interactions between water availability and crop development. The hydrological
303   model PCR-GLOBWB 2 is designed to simulate hydrological processes such as river
304   discharge, groundwater flow, and water storage dynamics. It provides detailed representation
305   and insights into the state and dynamics of water resources over large spatial scales and long
306   temporal scales. On the other hand, the crop growth model WOFOST is focused on simulating
307   crop phenology, including the stages of crop development, growth, and yield formation under
308   varying environmental conditions.

309   Despite the strengths of each model, they individually have limitations that can affect the
310   accuracy of simulations. PCR-GLOBWB 2 relies on static vegetation parameters, such as fixed
311   Leaf Area Index (LAI) and root depth, which can limit its ability to reflect the dynamic nature
312   of crop growth. On the other hand, WOFOST offers a detailed and dynamic representation of
313   crop phenology and development, adjusting parameters like LAI and root depth based on actual
314   growth stages. However, WOFOST employs a simplified water balance model, that may not
315   adequately capture complex hydrological interactions.

316   To address these limitations, it is important to combine the strengths of both models to enhance
317   hydrological and crop modelling performance. By integrating, WOFOST's detailed crop
318   growth simulation capabilities with the robust hydrological process simulations of PCR-
319   GLOBWB 2, we can better understand and represent the soil-plant-atmosphere interactions.
320   Therefore, this study integrates PCR-GLOBWB 2 and WOFOST by passing soil moisture data

from PCR-GLOBWB 2 to WOFOST and feeding vegetative fluxes from WOFOST back into PCR-GLOBWB 2 on a daily basis. Additionally, to understand the intricate dynamics between hydrology and crop model, PCR-GLOBWB 2 is coupled to the WOFOST in one-way and two-way interactions.

In evaluating various coupling methods for integrating hydrological and crop models, we identified several approaches, including one where the hydrological model directly provides detailed irrigation schedules and percolation rates to the crop model. While this method offers highly detailed hydrological inputs, it often leads to inconsistencies due to the separate handling of soil moisture dynamics between the models, resulting in errors in soil moisture management and water balance. Commonly used coupling procedures, such as those described by Li et al., (2014) and Tsarouchi et al., (2014), calculate potential evapotranspiration and vegetation water uptake within the hydrological model, which is then passed to the crop model to simulate crop growth. The crop model then calculates state variables like leaf area index, root depth, and canopy height, which are subsequently fed back into the hydrological model. However, these methods can introduce system errors, particularly in the transpiration module, if there is a discrepancy between evapotranspiration calculated by the crop and hydrological model, as highlighted by Wang et al., (2012). Our chosen coupling method, where soil moisture is calculated by PCR-GLOBWB 2 and passed to WOFOST and vegetative dynamics and evapotranspiration fluxes are then fed back into PCR-GLOBWB 2, offers a balanced approach that ensures consistency, and the necessary complexity, and efficiency in the simulations.

The selected coupling approach also addresses specific challenges associated with the models. PCR-GLOBWB 2 allows for flexible land cover classification and parameterization, which is essential for accurately representing diverse crop types and their interactions with water resources. For this study, we defined 12 land cover types (tall natural, short natural, pasture, irrigated maize, irrigated soybean, irrigated wheat, non-paddy irrigated crops (irrigated other crops), paddy irrigated crop, rainfed maize, rainfed soybean, rainfed wheat and rainfed others. WOFOST's role in this coupling is to pass the fluxes of irrigated and rainfed maize, soybean and wheat to PCR-GLOBWB 2, ensuring a detailed simulation of crop water use.

One of the key considerations in this coupling is accurately calculating the soil-water balance. Given its more advanced soil moisture accounting scheme, PCR-GLOBWB 2 handles this aspect, as WOFOST's simpler single-layer leaky bucket approach could introduce complexities if soil moisture data were passed from WOFOST to the multi-layered soil model

353 of PCR-GLOBWB 2. Therefore, the coupling approach we selected minimizes potential
354 discrepancies while maximizing the strengths of each model.

355 It is important to acknowledge, that individual models come with inherent uncertainties, related
356 to model structure, parameters and data. When coupling these models, the level of uncertainty
357 compounds further (Kanda et al., 2018). Additionally, the nature of coupling itself can
358 introduce another layer of uncertainty. According to Antle et al., (2001), coupling models lead
359 to further conceptualization and computational problems, elevating uncertainty levels.
360 Therefore, an efficient coupling is essential to minimize these risks. There are three primary
361 methods for coupling models (Vereecken et al., 2016): light/loose coupling,
362 external/framework coupling using a central coupler, and full coupling.

363 In light or loose coupling, the output of one model serves as the input for the other, which can
364 lead to a straightforward but limited interaction. Framework coupling uses a central coupler for
365 communication between models without requiring code modification, offering a balance
366 between integration and flexibility. Full coupling involves both models sharing the same
367 boundary conditions, drivers, and variables, which requires significant code modification.

368 **Implementation of the (BMI) framework coupling**

369 Given the complexity of integrating the PCR-GLOBWB 2 and WOFOST models and the need
370 for efficient simulations, we opted for framework coupling. This approach was chosen because
371 WOFOST and PCR-GLOBWB 2 are written in different programming languages (C and
372 PCRaster-Python, respectively). Framework coupling allows for seamless interaction between
373 the models at each time step, facilitating dynamic exchanges while limiting I/O-related
374 computation times. We employed the Basic Model Interface (BMI) for this purpose (Hutton et
375 al., 2020; Peckham et al., 2013). The decision to use BMI over alternative techniques was
376 driven by its non-interfering nature, ensuring no code entanglement and facilitating seamless
377 connection between the two models. BMI functions act as a bridge, enabling direct variable
378 exchange between WOFOST and PCR-GLOBWB 2 without modifying their source code. This
379 non-invasive approach ensures a flexible and robust coupling framework, allowing continuous
380 model development without interruptions. Integrating BMI functions into both models
381 provides a set of functions for retrieving or altering model variables, enhancing adaptability
382 and efficiency.

383 An additional wrapper was required to translate the model-specific BMI functions into Python-
384 compatible information to establish a Python-based coupling framework. The Babelizer

385 wrapper (CSDMS, 2024) was utilized for this purpose with the WOFOST BMI. Conversely,

386 no supplementary wrapper is needed in the PCR-GLOBWB 2 BMI, as the model is inherently

387 Python-compatible due to its programming language.

388 The Babelizer wrapper facilitates the integration of the WOFOST model by utilizing an input

389 file that provides essential details, including the model library, entry point, packages, and

390 author information. This input file guides the construction of the necessary dependencies to

391 generate Python bindings. Once these Python bindings are created, Babelizer ensures the

392 successful integration of the WOFOST BMI into Python by verifying that the bindings are

393 correctly built and loaded.

394 **Workflow of PCR-GLOBWB 2 - WOFOST model framework**

395 In the PCR-GLOBWB 2 - WOFOST coupling framework, the workflow after implementing

396 BMI functions remains consistent for both one-way and two-way coupling, up until the

397 initialization of the hydrological and crop models (Fig. 2).

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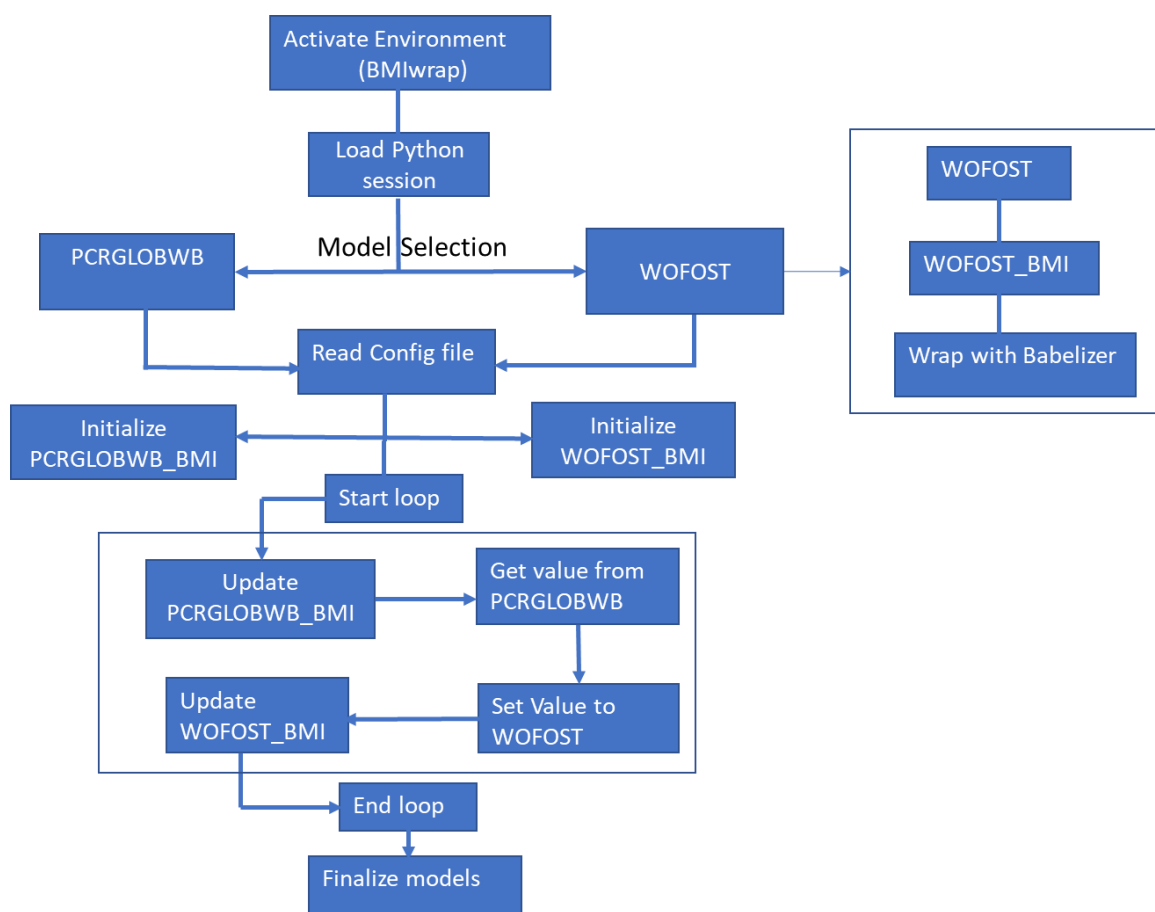
399 **Figure 2: Schematization of the workflow of the coupled PCR-GLOBWB 2 - WOFOST model framework**

Before initiating the Python session, it is crucial to activate the BMI wrap environment, which includes all necessary libraries for both hydrological and crop models. After this setup, the PCR-GLOBWB 2 and WOFOST models, along with their configuration files that define the coupling settings, are loaded into the Python session. BMIwrap reads the configuration file, initializing the model-specific configuration settings before establishing both models as a coupled entity.

Once the coupled models are initialized, a loop is initiated, commencing at the start time and concluding at the end time. During each iteration of this loop, variables are exchanged between the models based on the one-way or two-way coupling configuration. This iterative process ensures a continuous and seamless flow of information between the PCR-GLOBWB 2 hydrological model and the WOFOST crop model throughout the simulation period.

2.3.Model coupling setup

The developed 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 &3. 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.

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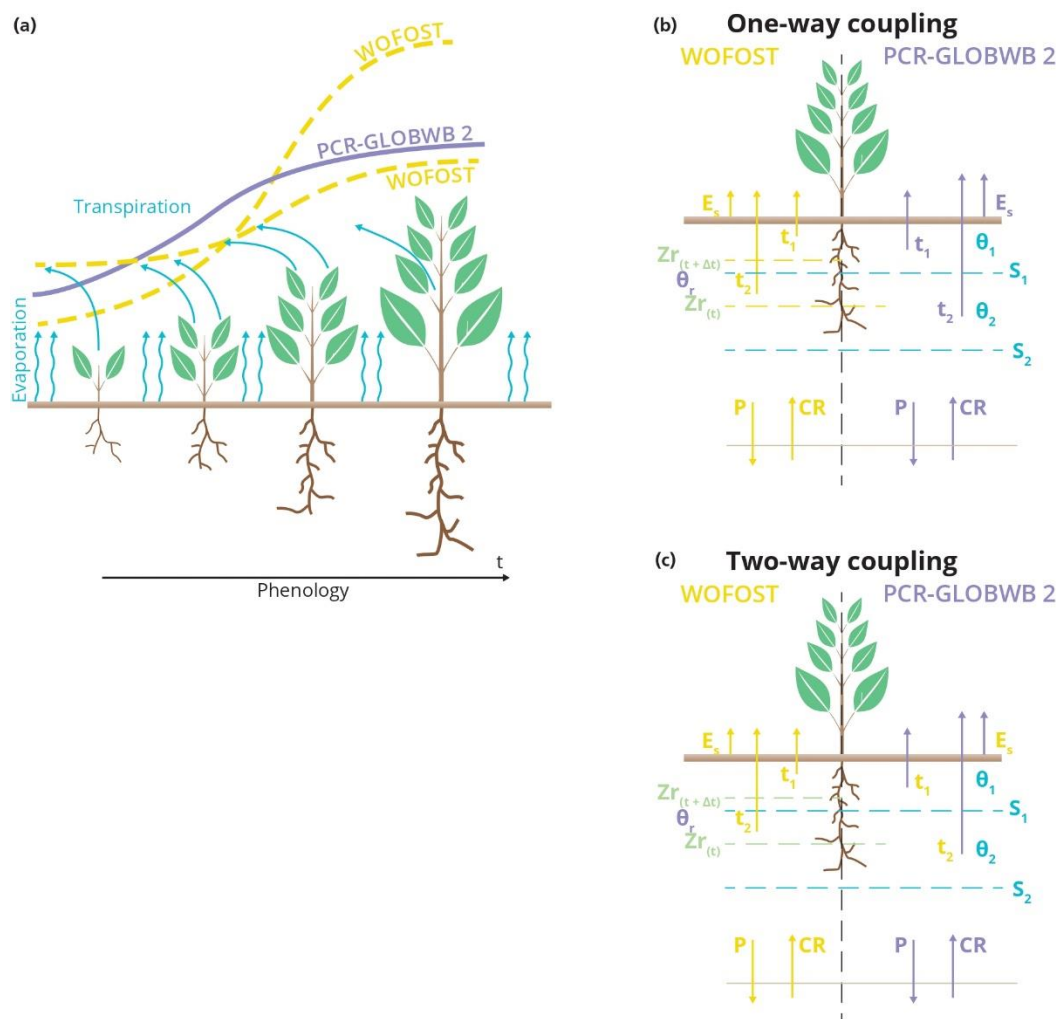
Figure 3: Schematic view of the coupled model framework: a) shows the calculated phenology from WOFOST and PCR-GLOBWB 2 over time along with the associated fluxes. b) displays a detailed representation of the one-way coupling approach, where ~~variables such as~~ soil moisture ~~are exchanged~~is transferred from PCR-GLOBWB 2 to WOFOST and (c) illustrates the two-way coupling approach, where variables are exchanged in both directions between PCR-GLOBWB 2 and WOFOST.

2.3.1. One-way coupling

In the one-way coupling, information on soil moisture status is passed from PCR-GLOBWB 2 to WOFOST (Fig 3(b)). 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.

2.3.2. Two-way coupling

- In addition to one-way coupling, the two-way coupling approach involves iterating data exchange between WOFOST and PCR-GLOBWB 2 twice per day. WOFOST calculates the vegetation states, (such as leaf area index (LAI), biomass and root depth) and fluxes (e.g., evapotranspiration) for irrigated and rainfed maize, soybean and wheat crops, while other vegetation and non-vegetation fluxes for other crops are simulated within PCR-GLOBWB 2. To be more specific, for the fraction of land cover that is different from maize, wheat and soybean, the vegetation states and fluxes are calculated within the PCR-GLOBWB 2. For these land cover types, vegetation phenology in the form of crop factors, is approximated by a yearly climatology. In the two-way coupling, data is exchanged between PCR-GLOBWB 2 and WOFOST as follows (Fig. 3c): At the start of the day, PCR-GLOBWB 2 passes the previous day's soil moisture to the WOFOST, assuming no root development has occurred overnight. WOFOST then computes the potential evapotranspiration based on the meteorological variables at the current time step and the pertinent vegetation states from the previous time step (leaf area index (LAI), rooting depth, and crop height). It also calculates the actual bare soil evaporation, actual transpiration (actual evapotranspiration), potential evaporation and open water evaporation;

- The calculated 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 forced to 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 in PCR-GLOBWB 2. 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 based on 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;

- At the end of the day, the resulting soil moisture from the two soil layers from PCR-GLOBWB 2 is aggregated to provide a total for the root zone of each crop, which is then passed back to WOFOST;

- Using the updated soil moisture from PCR-GLOBWB 2, WOFOST computes the actual transpiration and updates crop growth and the crop status. The new fluxes and crop parameters are then passed to PCR-GLOBWB 2 again on the next day (Fig.1, Fig. 3c).

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~~stand-alone) 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.

2.4. Model coupling simulation experiments and parametrization

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~~stand-alone 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~~stand-alone 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 IIIII.

Additionally, to ensure a consistent comparison, we harmonized the soil parameters in both WOFOST and PCR-GLOBWB 2 by incorporating data from the FAO soil map (FAO, 2007). WOFOST uses constant soil parameters across all spatial locations, which may not accurately represent local soil variability. By integrating FAO soil data, we ensured consistency in soil properties such as water-holding capacity and infiltration rates across the different models, improving the robustness of the comparison.

Comparisons were made between simulations from standalonestand-alone 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. Furthermore, irrigation water withdrawals of coupled model runs are compared against the USGS Water Use Database (USGS, 2023) (section 2.4).

2.5. 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.

2.5.1. 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.

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

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

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

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.

2.5.2. Irrigation water use model evaluation

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

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

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

578   **3. Results**

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

584   **3.1 Comparative temporal and spatial analysis of stand-alone, one-way, and two-way**
585   **coupling for irrigated and rainfed crops**

586   Temporal analysis (Fig. 2) compares the simulated yields with reported yields for irrigated and
587   rainfed maize, soybean, and wheat crops spanning from 1979 to 2019 in the CONUS region.
588   Notably, the reported yields exhibit discernible trends for the CONUS region across the three
589   crops and in both irrigated and rainfed analysis. This temporal evolution is primarily attributed
590   to technological advancements, encompassing improved agricultural practices and the

591   introduction of enhanced crop varieties over the study period (Arata et al., 2020). In contrast,
592   simulated yields of our coupled PCR-GLOBWB 2–WOFOST model framework do not capture
593   such trends, as the modelling approach intentionally omitted to incorporate trends in
594   technology and management practices. This intentional omission was to focus on the intrinsic
595   biophysical processes and climatic conditions affecting crop yields, providing a baseline
596   understanding unaffected by external advancements.

597   The trends in reported yields differ significantly across all crops and between irrigated and
598   rainfed systems. For maize, both irrigated and rainfed yields show an increasing trend,
599   particularly post-2000, which is not reflected in the simulated yields. Soybean yields exhibit a
600   gradual upward trend in irrigated systems, while rainfed soybean yields show little to no
601   discernible trend until 2007, followed by a slight increase. Wheat yields, both irrigated and
602   rainfed, demonstrate fluctuations with a slight upward trend towards the end of the period.
603   These discrepancies can be attributed to various factors, including technological advancements,
604   improved agricultural practices, and the introduction of enhanced crop varieties, which were
605   not incorporated into the modelling approach. To ensure a consistent and meaningful analysis,
606   we selected the years 2006-2019 for further analysis (spatial analysis (Fig. 5) and evaluation
607   metrics (Table. 1)). This period was selected because reported yields during these years appear
608   more stable and are better aligned with the simulated yields, allowing for a fair evaluation of
609   the model's accuracy and reliability. For the selected periods, we think that the results are
610   convincing, and, except for rainfed Soybean, they are certainly up to par with the results from
611   other crop growth modelling studies at continental scales.

612

613
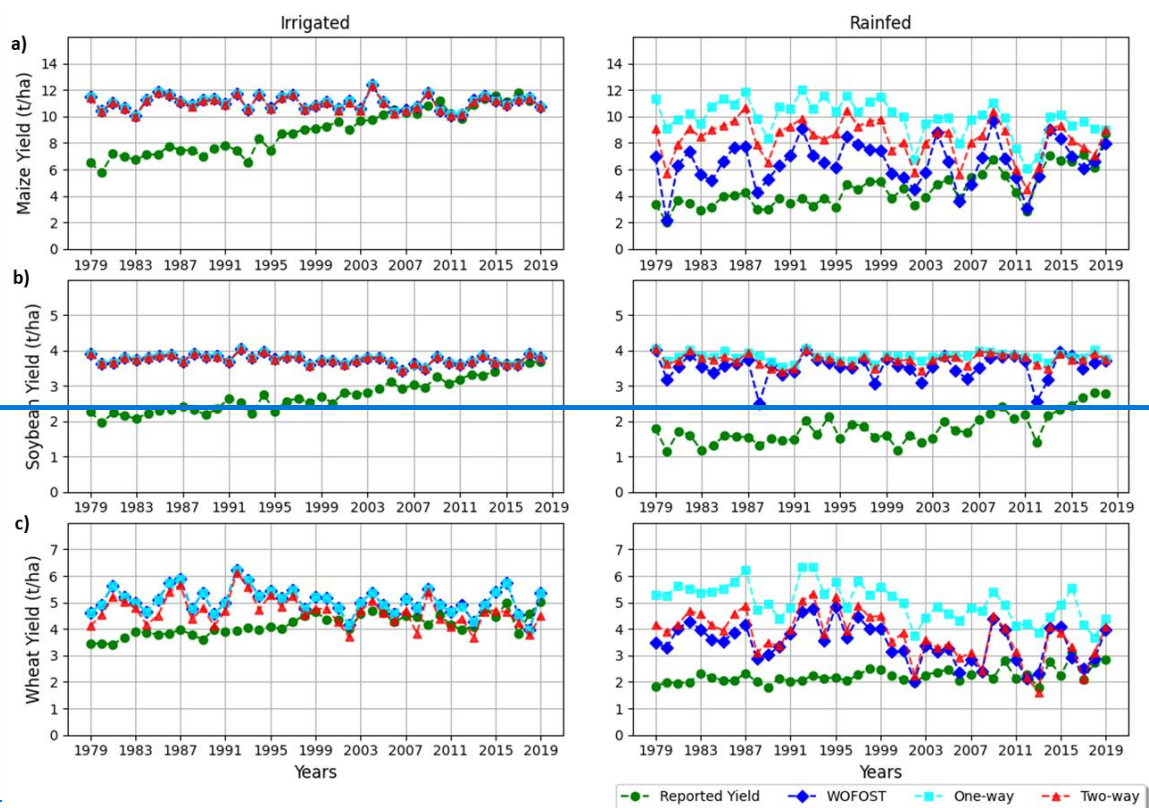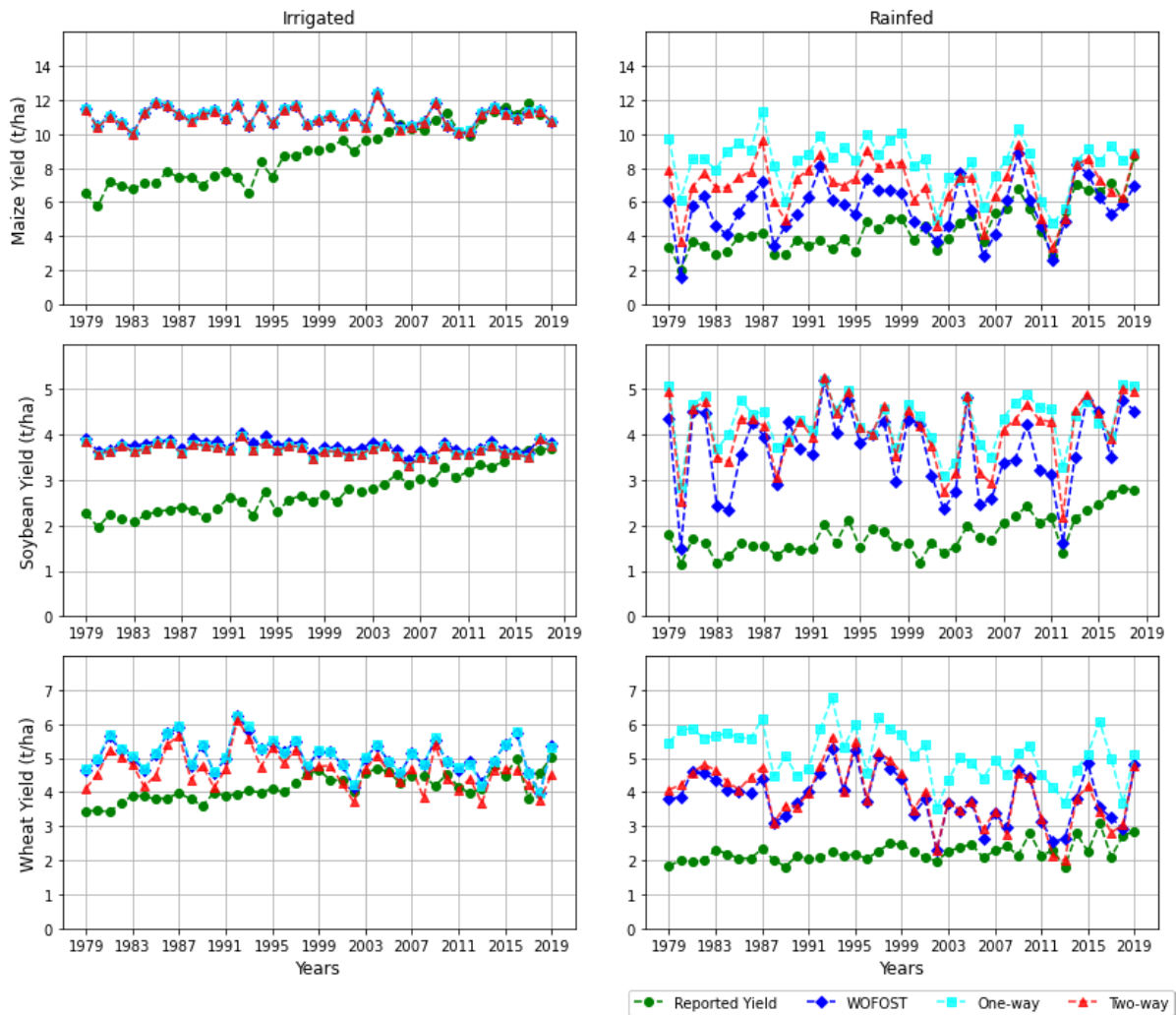
Figure 4: Temporal analysis of irrigated and rainfed crops of a) maize, b) soybean and c) wheat for the years 1979 to 2019 of a CONUS region

618
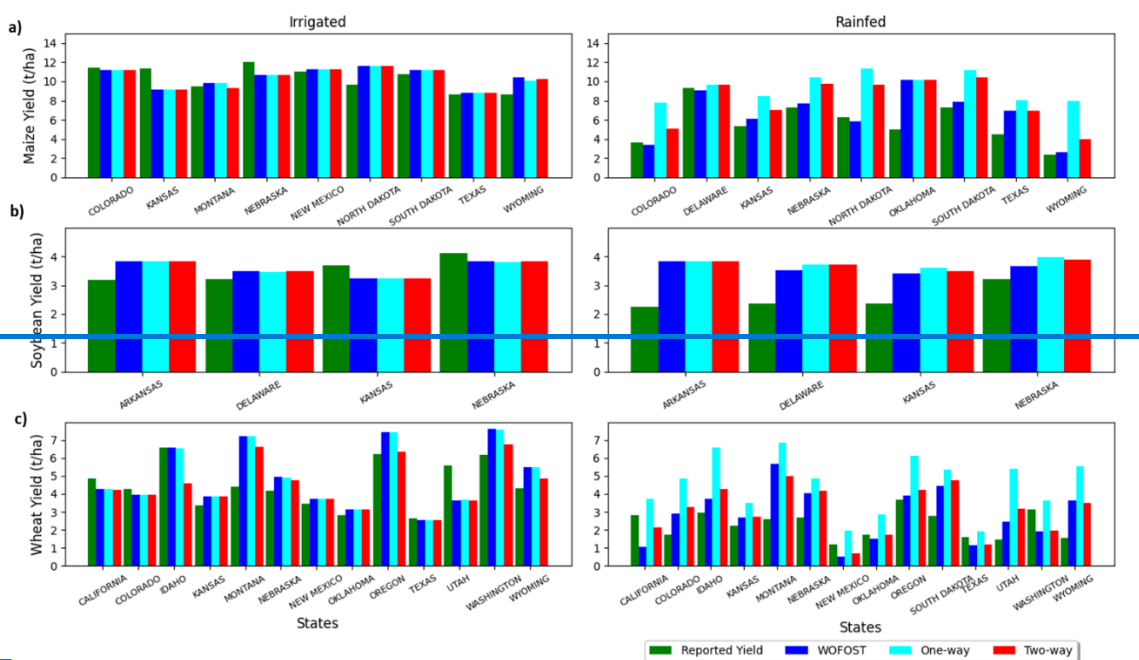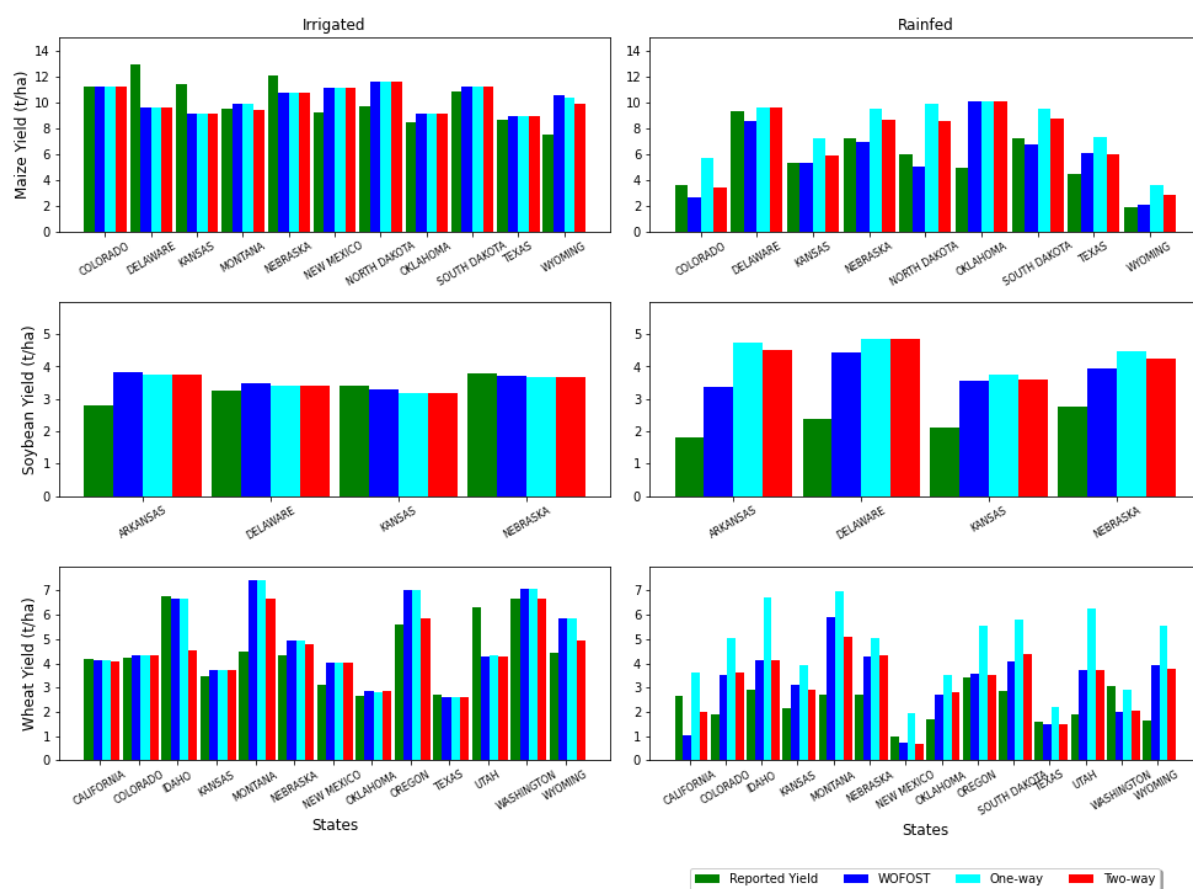
Figure 5: Spatial (i.e., state level) analysis of irrigated and rainfed crops of a) maize, b) soybean and c) wheat for the years 2006 to 2019 for the CONUS region.

Figures 4 and 5 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~~stand-alone 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~~stand-alone runs, indicating that there is generally enough irrigation water to completely satisfy crop water demands. This similarity arises because in irrigated conditions, water supply is managed to meet crop water demands fully, thereby minimizing the influence of soil moisture variability on yield outcomes. In other words, since the primary constraint, water availability, is alleviated by irrigation, the simulations naturally converge, regardless of the model coupling approach. 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 that rely solely on rainfall, we generally expect similar yields from stand-alone and two-way coupled simulations, since the primary water input, is rainfall. However, differences were observed between these models, ~~especially~~ more pronounced in maize crops and less significant in soybean and wheat~~,~~, with yields in the two-way coupled model being larger than stand-alone WOFOST. These ~~variations between the two models~~ differences can be attributed to various factors. The coupled model incorporates detailed soil moisture dynamics, including processes like ~~infiltration,~~ percolation, capillary rise and surface runoff, which directly influence water availability for crops. For example, higher ~~infiltration rates~~ capillary rise from groundwater can increase soil moisture, thereby increasing water available to crops, whereas ~~greater~~ surface runoff limits infiltration, and deep percolation rates ~~might~~ lead to water loss beyond the root zone, reducing available moisture. In contrast, ~~standalone~~ stand-alone WOFOST cannot accurately capture such variability, leading to differences in simulated yields. ~~Additionally, the coupled model integrates simulations of surface runoff and lateral water redistribution, which impact local soil moisture levels. In areas with significant runoff, less water infiltrates the soil, thereby reducing moisture availability for crops. This aspect is often simplified or omitted in standalone crop models, which might assume uniform water availability from rainfall. These differences contribute to the differences in simulated yields, with the coupled model providing a more comprehensive simulation of hydrological conditions affecting crop productivity~~.

Another key distinction lies in how the plants access soil moisture in the root zone in the different models. In the stand-alone WOFOST model, all soil moisture is extracted from a single soil layer using a simple one-layer tipping bucket approach. Conversely, PCR-GLOBWB 2 subdivides the soil profile into two layers (see section 2.1), with evapotranspiration distributed between them. In this setup, bare soil evaporation is entirely sourced from the upper layer, while transpiration is drawn from both layers. In the coupled approach, soil moisture can be disproportionately supplied from the wetter second layer, including the part of the second soil layer that is below the root zone. This provides slightly higher average root zone soil moisture to WOFOST under stressed conditions, making the simulated yields of the two-way-coupled PCR-GLOBWB 2- WOFOST a bit higher than those of stand-alone WOFOST (see Supplementary Information III-2, Supplementary Figure S7-S10 for a detailed analysis of the differences between stand-alone WOFOST, one-way and two-way coupled PCR-GLOBWB 2 – WOFOST models).

The one-way coupling approach ~~tended to exhibit an overestimation of~~generally overestimates 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~~ (Leaf area index and root development) is prescribed and independent of actual crop development as simulated by WOFOST. In a dry and warm year, crop development in WOFOST is faster than average and thus also faster than the fixed~~) which could, as described before, lead~~ development in PCR-GLOBWB 2; this is due to ~~an over-estimation of soil moisture availability that is then~~higher radiation and temperature at the beginning of the growing season. This leads to early-season higher evapotranspiration in the stand-alone WOFOST model and less available soil moisture at the end of the season when the storage organs are formed (see Supplementary Information III-1). In a one-way coupled setup, plant development from WOFOST is not fed back to PCR-GLOBWB 2, so that soil moisture in PCR-GLOBWB 2 remains higher throughout the season. This higher soil moisture is 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 and dynamically adjusts the root zone depth based on actual crop development stages. As a result, the two-way coupling approach results in more realistic soil moisture and~~ higher yields in the one-way coupled PCR-GLOBWB 2 – WOFOST model than the stand-alone WOFOST model and the two-way coupled PCR-GLOBWB 2 – WOFOST model, where crop ~~yield simulations.~~development is fed back to PCR-GLOBWB 2. We further refer to Supplementary Information III, Supplementary Figure S5-S10, for a detailed analysis of the differences between stand-alone WOFOST, one-way and two-way coupled PCR-GLOBWB 2 – WOFOST models.

The temporal analysis (Fig. 4) of simulated and reported yields reveals distinct trends and year-to-year fluctuations for each crop. For maize, both irrigated and rainfed conditions show considerable variability in yields over the years. Rainfed maize, in particular, exhibits a discernible pattern with certain years marked by notable peaks in yields, highlighting its sensitivity to varying environmental conditions. These variations are also observed in reported maize yields. This indicates that maize yields, especially under rainfed conditions, are highly influenced by annual climatic variability.

For wheat, the simulated yields under both irrigated and rainfed conditions show similar year-to-year patterns, which are not as evident in the reported yields. This suggests that the

699 discrepancies might be due to the model's sensitivity to water and temperature variability,
700 which may not fully capture the complexities of actual wheat production. Specifically, factors
701 such as the use of different wheat varieties, the differentiation between winter and spring wheat,
702 and their respective growth parameters could influence the observed yields. These varietal and
703 seasonal distinctions introduce variability that the model might not fully incorporate, leading
704 to differences between simulated and reported yields.

705 Soybean yields present a different scenario. Both irrigated and rainfed simulated yields
706 consistently surpass the reported values, with the discrepancy being more pronounced in
707 rainfed conditions. This overestimation could be due to the model's assumptions or parameters
708 that do not fully capture the limitations faced by soybean crops in real-world rainfed
709 environments, such as variations in soil fertility, pest pressures, crop varieties and other
710 management practices not accounted for in the model.

711 In the spatial analysis (Fig. 5), simulated irrigated maize yields from stand-alone (WOFOST),
712 one-way, and two-way coupling align almost identical with reported irrigated maize yields.
713 Conversely, in rainfed maize analysis, both stand-alone and two-way simulations
714 ~~outperform~~closely matched reported yields in states such as Delaware, Colorado, Kansas,
715 ~~North~~Nebraska, South Dakota~~,~~ and Wyoming, while one-way coupling exhibits an
716 overestimation of yields compared to stand-alone (WOFOST) and two-way coupling.

717 For soybeans, the spatial analysis reveals identical yields among stand-alone (WOFOST), one-
718 way, and two-way simulations for both irrigated and rainfed crops. For irrigated crops,
719 simulated yields were overestimated in Arkansas state but closely matched in states like
720 ~~Arkansas and~~ Delaware ~~and underestimated in,~~ Kansas and Nebraska compared to reported
721 values. Under rainfed conditions, all three models overestimated the simulated yield relative to
722 reported yields. For irrigated ~~and rainfed~~ wheat, simulated yields of the two-way coupling
723 outperform stand-alone WOFOST and one-way coupling, particularly in states like ~~Idaho,~~
724 ~~Montana, Oregon, and Wyoming.~~Oregon, Washington and Wyoming. In contrast, for rainfed
725 wheat, stand-alone and two-way coupling simulations closely align except in states such as
726 California and Montana. The one-way coupling, lacking feedback from the crop growth model
727 to the hydrological model, leads to an overestimation of rainfed yields across all states
728 compared to stand-alone WOFOST and two-way coupling. This underscores the importance of
729 incorporating two-way interactions and feedback mechanisms for more accurate yield
730 simulation results.

3.2 Evaluation statistics

Table 1 presents model performance metrics (correlation, normalized RMSE and normalized bias~~),~~) from the temporal analysis, evaluating simulations for the three model setups (i.e., ~~standalone~~stand-alone WOFOST, one-way, two-way coupling) for irrigated and rainfed maize, soybean, and wheat~~.~~ for the period 2006-2019 (see section 3.1). Model performance metrics for the spatial analysis are presented in supplementary IV.

For irrigated crops, ~~simulation~~simulations of all model approaches exhibit positive correlations~~. Specifically, for maize, the~~ with reported yields, though correlation coefficients ~~are high (0.63), moderate for soybean~~vary across models and ~~rather low~~crops. Two-way coupling shows a slightly higher correlation (0.59) with reported yields for maize, but a lower correlation (0.24) for wheat~~.~~ compared to stand-alone and one-way coupling. The ~~normalized~~ root mean square errors (RMSE) normalized to the mean remain consistently low, with values ranging from 0.~~13~~08 to 0.~~18~~15 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~~65 to 0.~~20~~50. The two-way coupling demonstrates overall slightly lower biases and minimal error 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~~57	0.~~63~~56	0.~~63~~59	0.~~46~~25	0.~~46~~36	0.~~45~~36	0.~~22~~45	0.~~22~~46	0.24
2	Normalized RMSE	0.~~13~~08	0.~~13~~08	0.~~13~~08	0.~~06~~12	0.~~06~~10	0.~~06~~10	0.~~18~~15	0.~~18~~15	0.~~18~~11
3	Normalized Bias	-0.~~20~~58	-0.2058	-0.~~20~~65	0.~~01~~34	0.~~01~~27	0.~~01~~27	0.~~12~~50	0.~~12~~50	-0.~~06~~02
Rainfed crops										
1	Correlation	0.~~77~~80	0.~~65~~81	0.~~77~~84	0.~~57~~86	0.~~22~~80	0.~~33~~84	0.~~44~~37	0.~~51~~46	0.~~55~~47

| 2 | Normalized RMSE | 0.2219 | 0.50 | 0.5020 | 0.4268 | 0.571.01 | 0.5791 | 0.3756 | 0.6697 | 0.6655 |
| 3 | Normalized Bias | -0.3410 | 1.652.00 | 0.8491 | 0.421.39 | 0.782.24 | 0.632.03 | 0.281.13 | 0.912.26 | 0.3298 |

For rainfed crops, the correlation coefficients vary, with two-way coupling displaying the highest correlations. Higher correlation coefficients are obtained for maize (0.65808-0.7784) and soybean (0.84-0.86) compared to soybean (0.22-0.57) and wheat (0.4437-0.5547). Normalized RMSE values are generally higher in rainfed conditions compared to irrigated, ranging from 0.2219 to 0.661.01. Normalized biases show variations across simulation approaches and crops, ranging from -0.2810 to 1.652.26. Specifically, one-way coupling exhibits higher biases in rainfed maize, soybean and wheat compared to stand-alone and two-way simulations. Two-way coupling shows lower error in wheat crops compared to the stand-alone model, while the stand-alone model performs better for maize and soybeans than both two-way and one-way coupling.

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.

Spatial patterns of the 1979-2019 mean simulated crop yields of maize, soybean and wheat are shown under irrigated (Fig. 6) and rainfed (Fig. 7) conditions across the CONUS region. The stand-alone simulations show the yield distribution without coupling between the hydrological and crop models, relying on the internal soil moisture calculation using a simple one-layer tipping bucket approach. In contrast, one-way and two-way coupled simulations involve dynamic interaction between the hydrological model (PCR-GLOBWB 2) and crop growth model (WOFOST), where soil moisture from PCR-GLOBWB 2 is passed to the WOFOST,

782 with two-way coupling also incorporating feedback from WOFOST to the PCR-GLOBWB 2.

783 (see Fig 3).

784 For irrigated crops (Fig. 6), the regions show similar yields for stand-alone, one-way and two-

785 way coupled simulations. This is expected since soil moisture is kept at optimal levels in

786 irrigated conditions, ensuring that water availability does not become a limiting factor.

787 Consequently, in one-way coupling, the feedback from ~~WOFOST to~~ PCR-GLOBWB 2 to

788 WOFOST is inconsequential, as the continuous supply of water minimizes the need for

789 dynamic interaction between the models.

790 For rainfed conditions (Fig. 7), where water availability relies on green water~~, the~~ only, crop

791 yields are comparatively lower than ~~in~~under irrigated conditions. Differences between the

792 various stand-alone, one-way and two-way coupling approaches become apparent, particularly

793 in the western part of the CONUS. Notable differences in yields between stand-alone and two-

794 way coupling simulations are observed in maize and wheat crops, both under irrigated and

795 rainfed conditions. However, these differences are more pronounced ~~in~~for rainfed crops~~,~~ (see

796 supplementary Fig S13), where water availability is a crucial factor influencing crop yields. In

797 the case of rainfed ~~soybean yields, there is a clear distinction between stand-alone and coupled~~

798 ~~models, especially in the northern and southern regions of the eastern CONUS. The stand-alone~~

799 ~~model's tendency to overpredict yields in rainfed conditions underscores the limitation of using~~

800 ~~a simple one-layer leaky bucket approach in regions where water availability is crucial for crop~~

801 ~~growth~~soybeans, differences were less evident in all the models.

802 ~~Notably, one~~One-way coupling ~~tends to simulate~~generally simulates higher yields for maize

803 and wheat compared to two-way coupling~~. This~~ (see Fig 7). As described in Section 3.1 and

804 Supplementary Information III, this discrepancy arises from the transmission of soil moisture

805 from the hydrological model to the crop growth model in one-way coupling, without receiving

806 feedback from crop development to the hydrological model. ~~As stated before (3.1), this may~~

807 ~~overestimate~~This leads to an overestimation of late-season soil moisture availability under drier

808 conditions subsequently leading to a likely overestimation of simulated crop yield by the one-

809 way coupling. Clearly, this feedback is more important in the western part of CONUS, which

810 is likely related to larger interannual climate variability (with more dry conditions) compared

811 to the eastern part (see the section hereafter). The larger differences in mean yields for rainfed

812 crops, particularly in the western CONUS, that occur between one-way and two-way coupled

813 simulations are further illustrated by looking at the relative differences between the two
814 coupling methods (see Supplementary Information IVV; Fig. S5S11).

815 ~~Additionally, the two-way coupling reveals that during dry spells, the interaction between~~
816 ~~declining soil moisture and crop growth leads to an earlier onset of crop stress. In contrast, one-~~
817 ~~way coupling which does not account for feedback from crop stress to soil moisture, tends to~~
818 ~~overestimate the severity and timing of water stress on crops. In the two way coupled~~
819 ~~simulations, the slower crop development due to water stress in dry years feeds back into the~~
820 ~~hydrological cycle by reducing evapotranspiration rates. This reduction in evapotranspiration~~
821 ~~helps conserve soil moisture, thereby influencing the hydrological model's predictions of soil~~
822 ~~moisture availability. Such feedbacks are absent in one way coupling, where the fixed~~
823 ~~phenology leads to an overestimation of water uptake by crops, further exaggerating yield~~
824 ~~estimates. In some regions of the western CONUS, one-way coupling underestimates yields~~
825 ~~for rainfed crops of maize and wheat compared to two-way coupling, as the crop growth model~~
826 ~~WOFOST does not influence hydrological processes in the one-way coupling.~~

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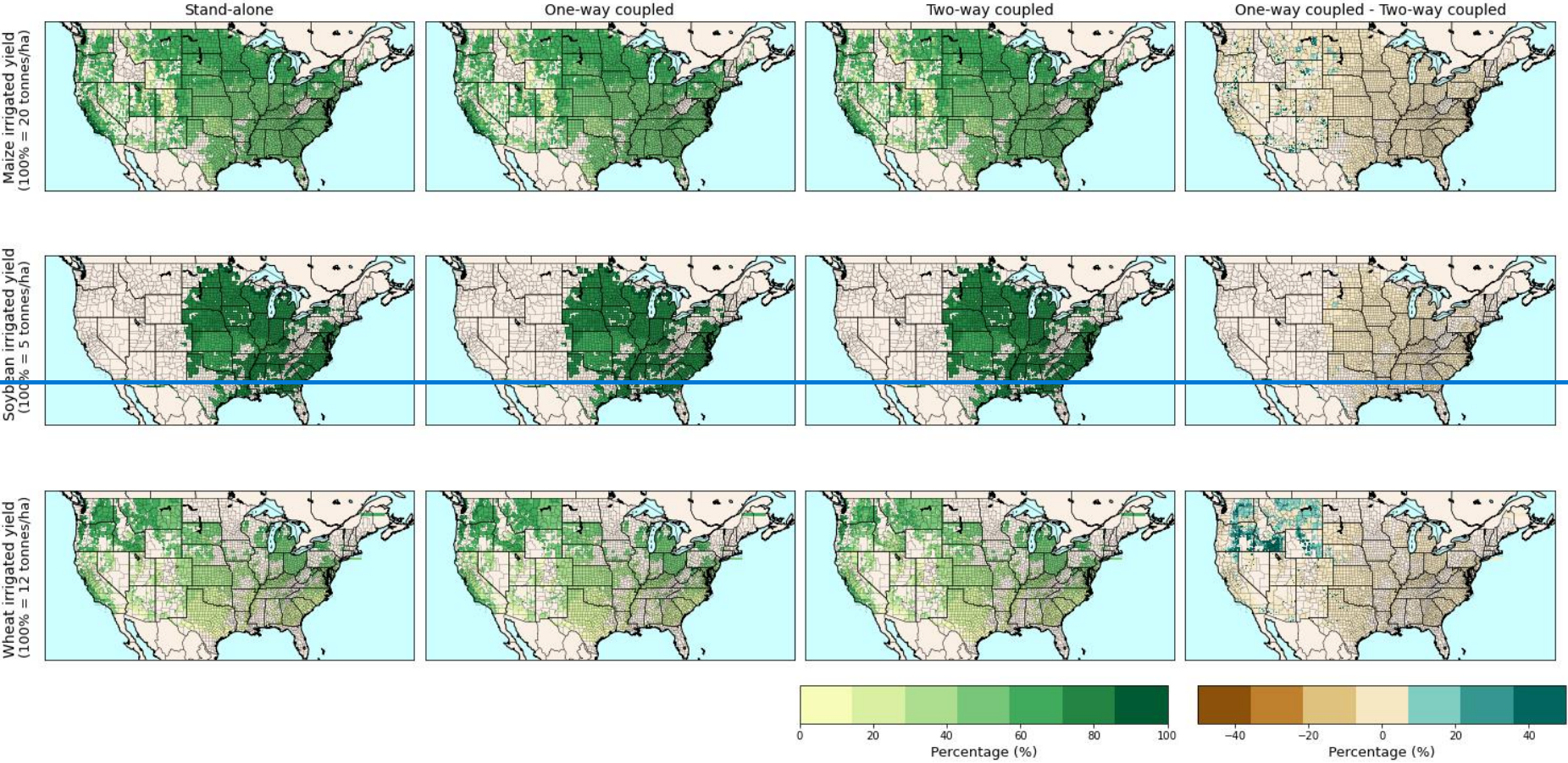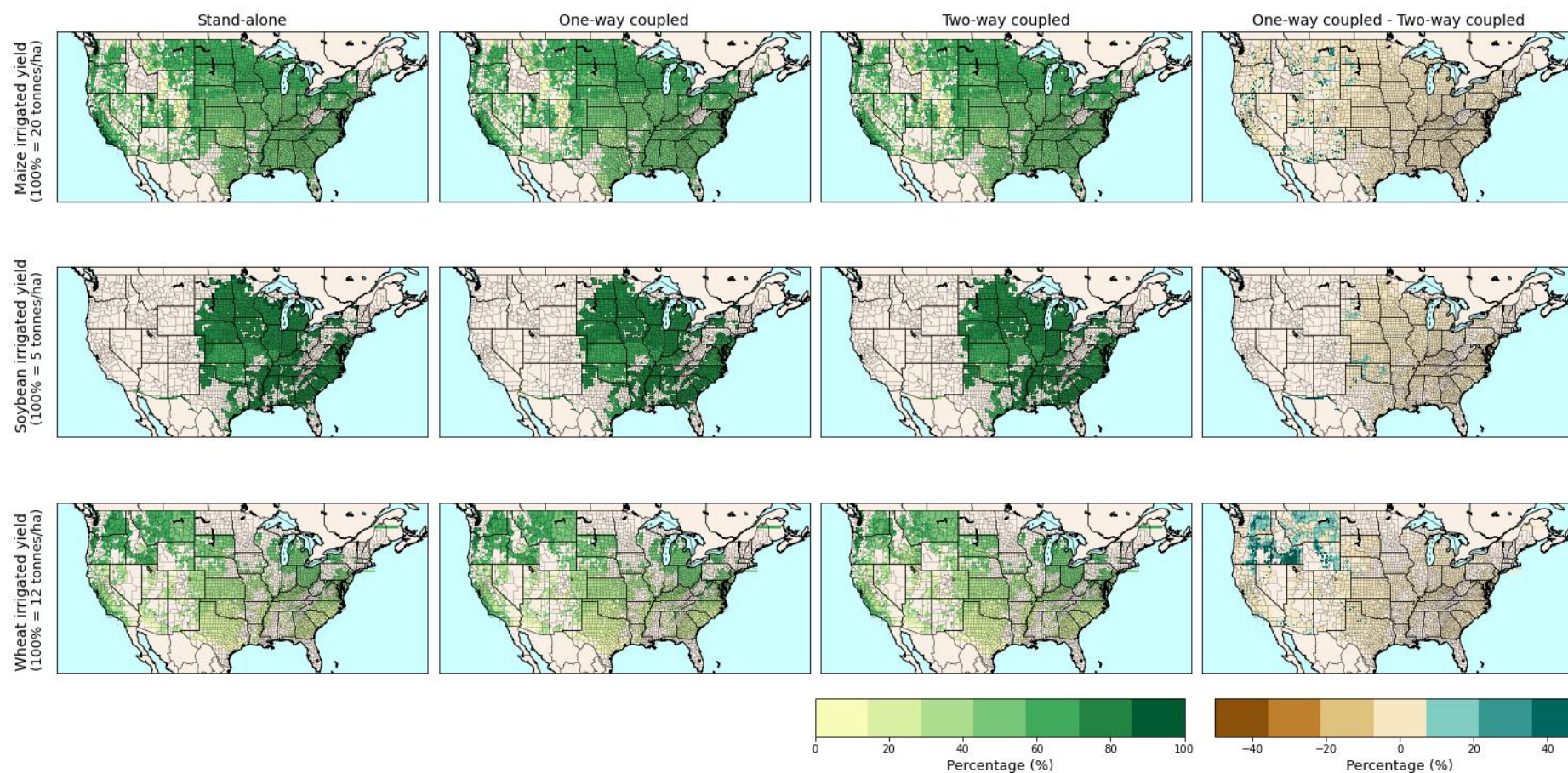
Figure 6: Mean irrigated crop yields for maize, soybean, and wheat within CONUS as obtained from stand-alone, one-way and two-way coupled simulations and differences between one-way and two-way coupled simulations for 1979-2019. Legend in % of values shown on the y-axes.

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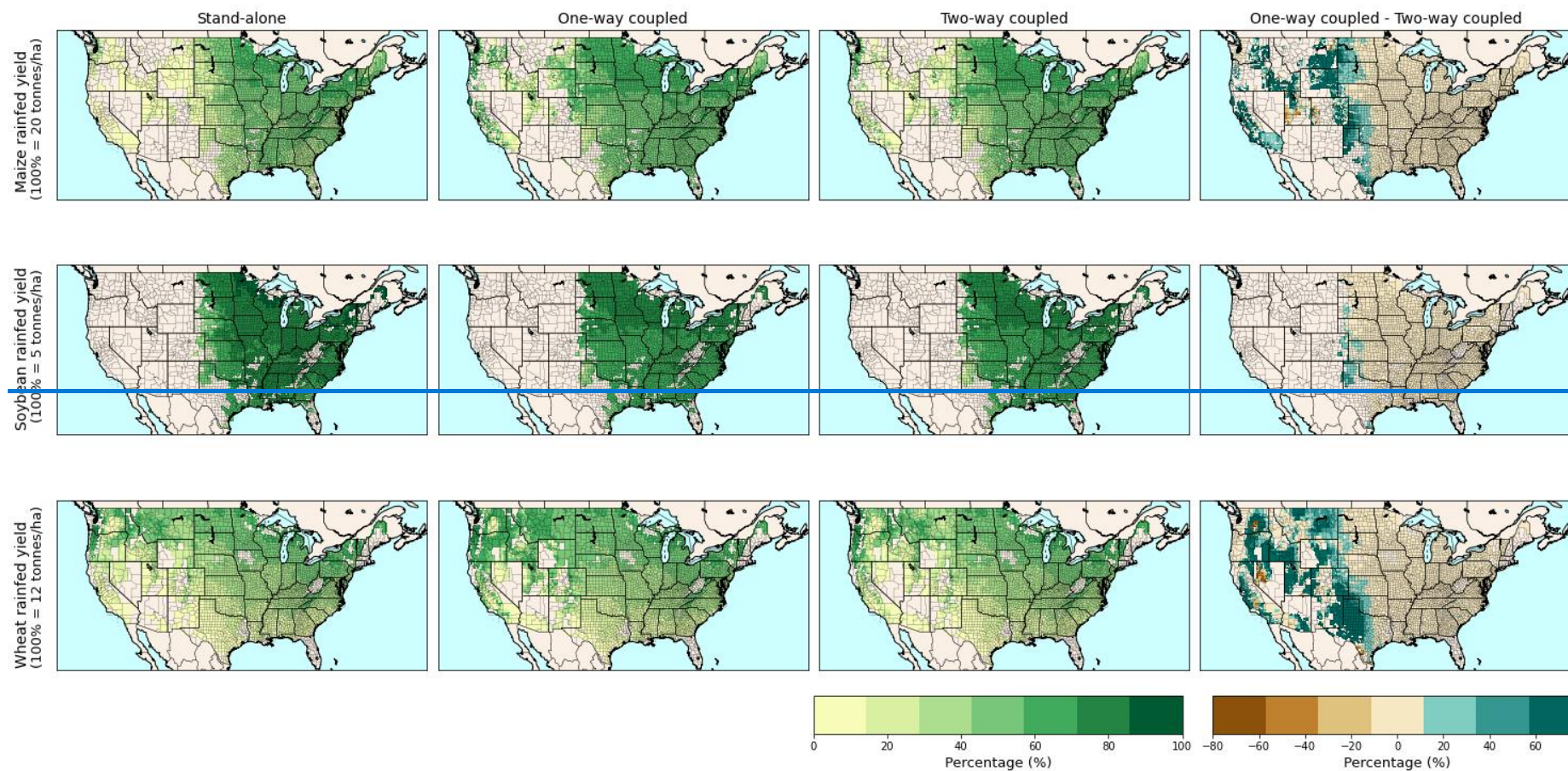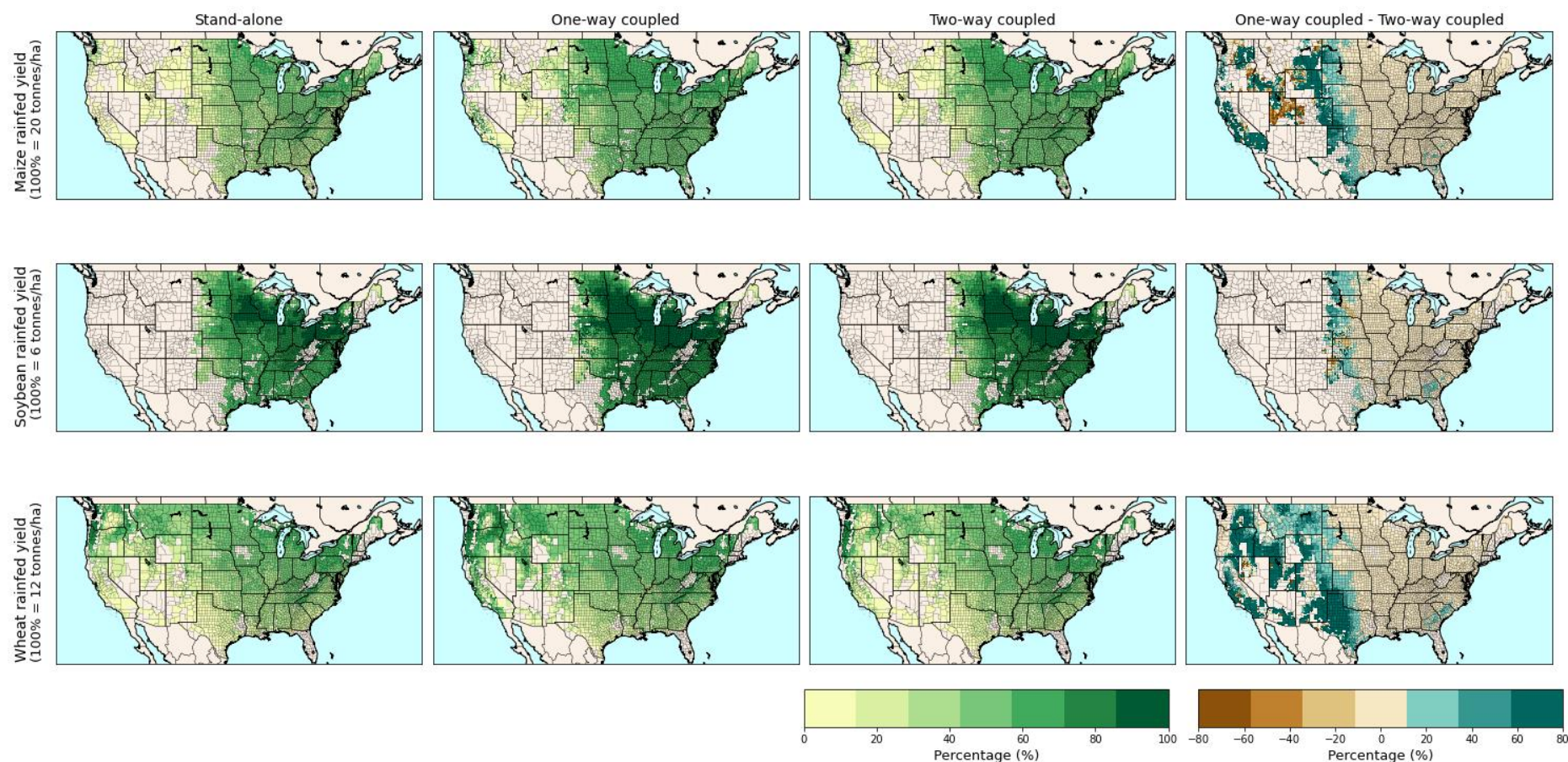
Figure 7: Mean rainfed crop yields for maize, soybean, and wheat within CONUS as obtained from stand-alone, one-way and two-way coupled simulations and differences between one-way and two-way coupled simulation for 1979-2019. Legend in % of values shown on the y-axes.

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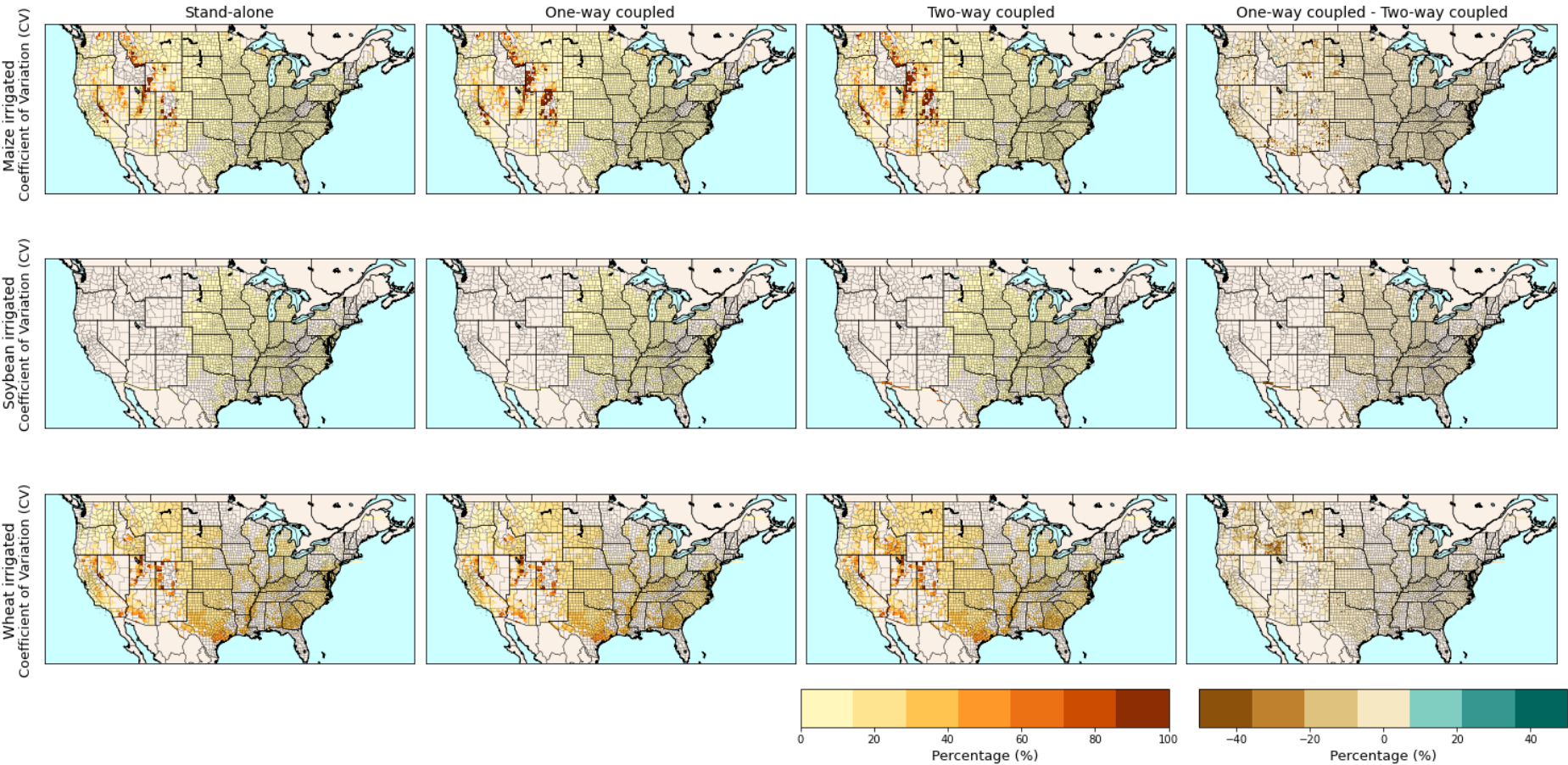
Figure 8: Coefficient of Variation (CV) over 1979-2019 of irrigated crop yields for maize, soybean, and wheat within CONUS as obtained under stand-alone, one-way and two-way coupling and difference between one-way and two-way coupling.

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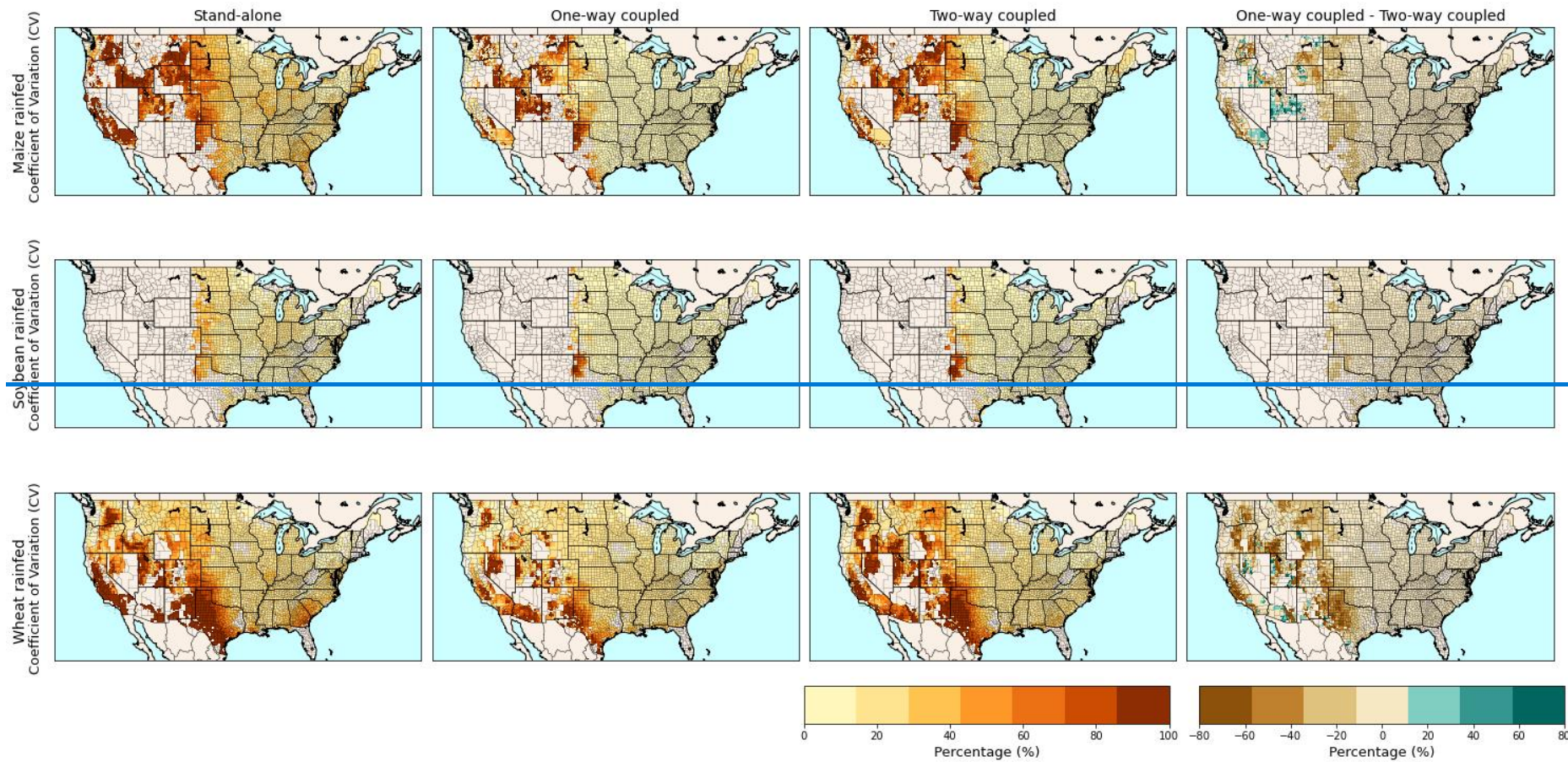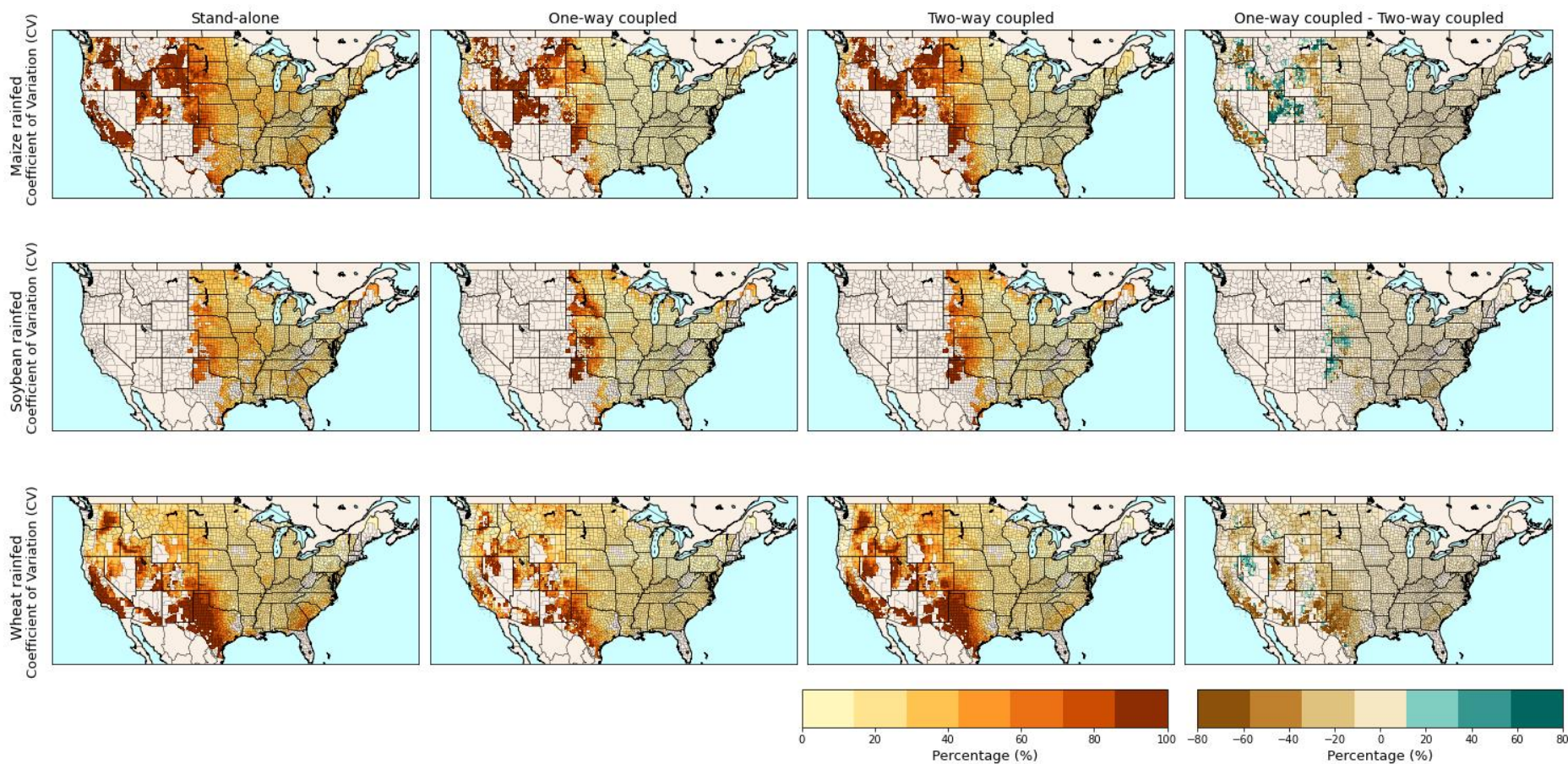
Figure 9: Coefficient of Variation (CV) over 1979-2019 of rainfed crop yields for maize, soybean, and wheat within CONUS as obtained under stand-alone, one-way and two-way coupling and difference between one-way and two-way coupling.

Spatial patterns of the coefficient of variation (CV) (in % of the mean) across CONUS for maize, soybean and wheat are shown under irrigated (Fig. 8) and rainfed conditions (Fig. 9) comparing the simulations of the stand-alone, 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~~V Fig. ~~S6~~S12, the differences between one-way and two-way coupled runs are generally small, except for some northwestern states.

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. 9). 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~~V Fig. ~~S6~~S12 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 7.

3.4 Irrigation water use

The scatter plot (Fig. 10) shows the relationship between reported USGS (after correction for area and irrigation efficiency – see 2.5.2) 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. 11) 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.

Figures 10 and 11 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

886 detailed crop cover data, irrigation efficacies and meteorological forcing than currently used in

887 the global version of PCR-GLOBWB 2.

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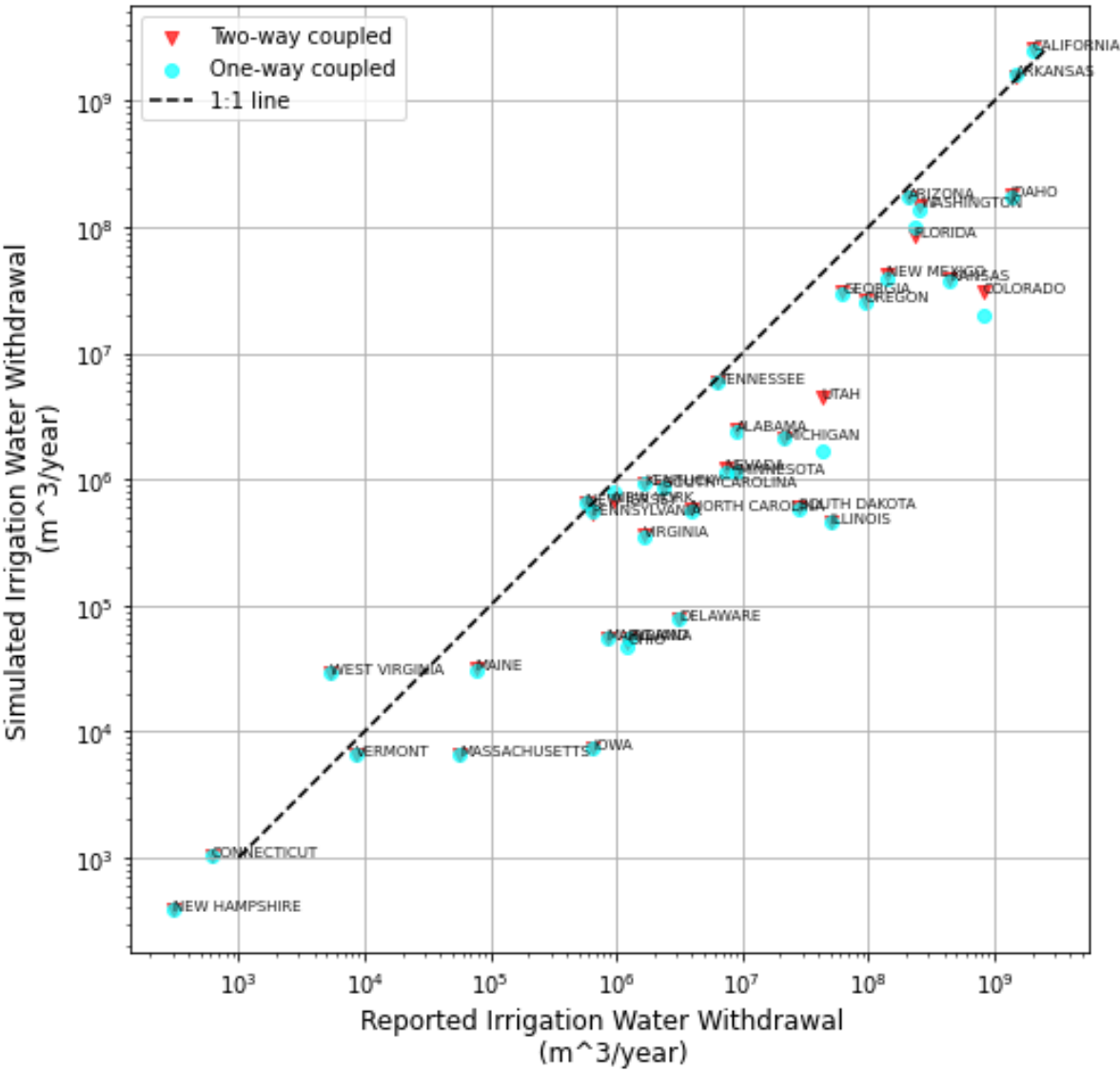
Figure 10: Spatial variation of one-way and two-way irrigation water withdrawal compared with USGS-reported water withdrawal data per state for all crops across the CONUS region with a logarithmic scale

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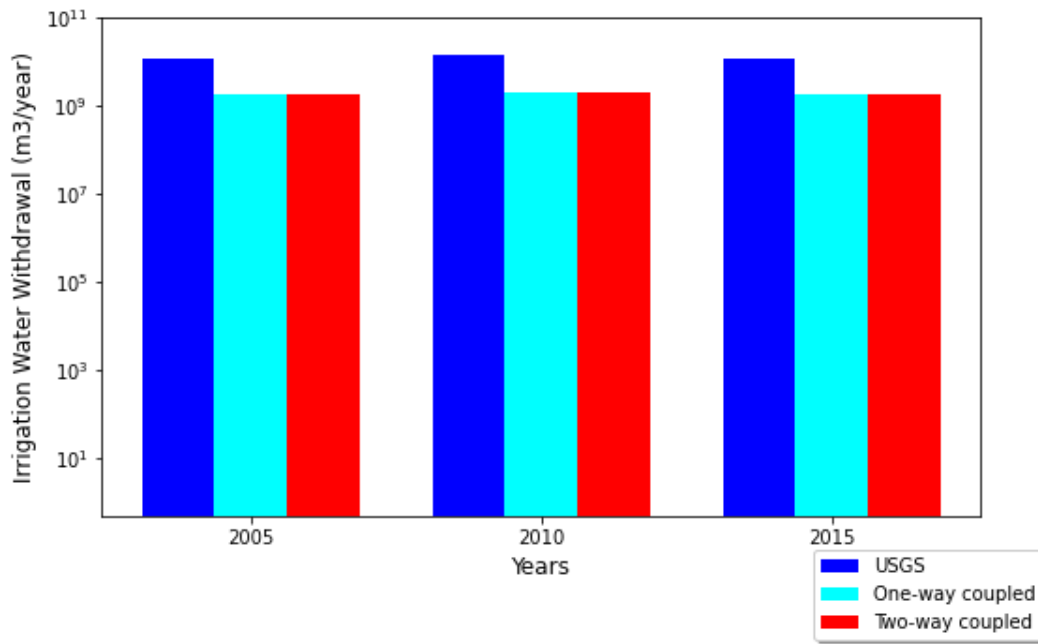
Figure 11: Temporal variation of one-way and two-way irrigation water withdrawal compared with USGS water withdrawal data of 5-year intervals across the CONUS region with a logarithmic scale.

4 Discussion and Conclusion

In this study, we developed a coupled hydrological-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 hydrological-crop growth modelling.~~

We hypothesized that a more realistic representation of soil moisture dynamics and water availability will lead to better estimates of water stress and yield outcomes. Validation against reported yields however did not show a notable improvement compared to the stand-alone WOFOST, both for rainfed as well as for irrigated agriculture. Thus, if the focus is on yield only, coupling with a hydrological model such as PCR-GLOBWB 2 seems not needed. However, although not picked up by the validation exercise, the coupling still allows the

913 inclusion of the impact of limited irrigation water availability as well as the impact of crop

914 development on the hydrological system. Our study also shows that if the focus is on these

915 impacts, it is necessary to use a two-way coupling to make sure that crop developments feeds

916 back on evaporation and soil moisture.

917

918 Another hypothesis we tested is whether integrating real-time crop growth information into

919 hydrological models will enhance the accuracy of predictions regarding irrigation needs and

920 water resource allocation. Although it can be expected that feeding back crop information to

921 PCR-GLOBWB 2 in the two-way coupling would improve estimates of irrigation water

922 withdrawal, this could not be substantiated by comparison with reported water withdrawal

923 statistics. One possible explanation is the use of constant crop area data across all years, which

924 introduces uncertainties and limits the model's responsiveness to actual land-use dynamics.

925 The spatiotemporal analysis of hydrological impacts on crop growth confirms the results shown

926 from the comparison with reported values. Notably, for rainfed crops, the estimated yield is

927 mostly higher for one-way coupled simulations compared to two-way and stand-alone

928 simulations. Also, the inter-annual variation of yield, that is, the sensitivity to drier and wetter

929 years, is notably higher for the two-way coupled and stand-alone simulations than the one-way

930 coupled simulations. This suggests that for a correct sensitivity to drought, a two-way coupling

931 that includes the feedback of crop status to the hydrological system is needed.

932 Our studies adds to previous work by Droppers et al., (2021), which investigated worldwide

933 water constraints and sustainable irrigation by coupling the Variable Infiltration Capacity

934 (VIC) hydrological model with WOFOST and Zhang et al. (2021) who focused on refining the

935 coupled VIC hydrological model with a crop growth model EPIC by incorporating the

936 evapotranspiration module at a regional scale. In comparison, our research extends the analysis

937 to a finer spatial scale and places a stronger emphasis on the comprehensive integration of

938 feedback loops between hydrology and crop growth. Particularly, we demonstrate the

939 importance of two-way coupling in capturing realistic yield outcomes, which is particularly

940 evident for rainfed crops. This is mainly because the two-way coupled system addresses the

941 influence of crop status on evapotranspiration and rooting depth, thereby impacting soil

942 moisture content, which in turn feed backs on crop growth. The two-way coupling approach

943 provides a more realistic depiction of water availability for crops, which results in larger inter-

944 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 (see section 3.2) 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 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 hydrological-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, This becomes evident when comparing yield estimates with observations over time (section 3.1; Fig. ~~2). The ignorance of technological innovations may contribute to discrepancies between simulated and actual yields.~~4).

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 hydrological-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. ~~Additionally, within the nexus context, the developed coupled framework can be integrated into various models across different programming languages, providing a flexible and adaptable tool to address a wide range of research needs.~~

In conclusion, the development and application of the two-way coupled hydrological-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~~Although it does not show an improvement of yield estimates per se, the coupling framework ~~not only~~ enhances our understanding of the interplay between hydrology and crop growth~~but~~. Also, through the sectoral water use modules of PCR-GLOBWB 2, ~~has~~it contains 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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