

1 **Process-based modeling framework for sustainable irrigation**  
2 **management at the regional scale: Integrating rice production, water**  
3 **use, and greenhouse gas emissions**

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## Abstract

Rice cultivation faces multiple challenges of rising food demand while increasing water scarcity and greenhouse gas emissions, intensifying the tension of the food-water-climate nexus. Process-based modeling ~~of the nexus~~ is pivotal for developing effective measures to ~~address-balance~~ these challenges. However, current models struggle to simulate their complex relationships under different water management schemes, primarily due to inadequate representation of critical physiological effects and ~~the absence-of~~ ~~lack of~~ efficient spatially explicit modeling strategies. Here, we propose an advancing framework that addresses these problems by integrating a process-based soil-crop model with vital physiological effects, a novel method for model upscaling, and the NSGA-II multi-objective optimization algorithm at a parallel computing platform. Applying the framework accounted for 52%, 60%, 37%, and 94% of the experimentally observed variations in rice yield, irrigation water use, ~~and~~ methane and nitrous oxide emissions in response to irrigation schemes. Compared with the origin model using traditional parameter upscaling methods, the advancing framework significantly reduced simulation errors by 35%–85%. Moreover, it well reproduced the multivariable synergies and tradeoffs observed in China's rice fields and identified additional 18% areas feasible for irrigation optimization, along with an additional 11% and 14% reduction potentials of water use and methane emissions, without compromising production. Over 90% of the potentials could be realized at the cost of 4% less yield increase and 25% higher nitrous oxide emissions under multiple objectives. Overall, this study provides a valuable tool for multi-objective optimization of rice irrigation schemes at a large scale. The advancing framework also has implications for other process-based modelling improvements efforts.

## Key points

- This study significantly improved rice yield simulations under various irrigation schemes by ~~quantifying and~~ incorporating critical physiological processes into a process-based model.
- This study developed a novel upscaling method of model parameterization that well reproduced observed synergies and tradeoffs among multiple objectives (i.e., rice yield, irrigation water use, methane emissions, and nitrous oxide emissions).
- This study provides a practical tool for multi-objective optimization of water management to deliver co-benefits of ensuring food production, saving water, and reducing greenhouse gas emissions of rice fields.

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## 1 Introduction

Rice is the staple food for more than half of the world's population and is also the most water-intensive cereal crop with a significant contribution to greenhouse gas emissions (GHGs) (Lampayan et al., 2015; Carlson et al., 2017). Rice cultivation currently accounts for 40% of global irrigation water use (IRR), 30% of methane (CH<sub>4</sub>), and 11% of nitrous oxide (N<sub>2</sub>O) emissions in agriculture (Yuan et al., 2021). To meet the demand of the growing population, a 50-60% increase in global rice production along with a 15% increase in water use are required by 2050, potentially leading to higher greenhouse gas emissions and intensifying the food-water-climate tensions of rice fields (Flörke et al., 2018). Therefore, ensuring food security while conserving water resources and reducing GHGs in rice cultivation is essential for achieving multiple United Nations Sustainable Development Goals.

Optimizing water management is promising to address the multiple challenges. However, different water management schemes can lead to a wide range of outcomes in rice yield (-16.9% to 21.9%), IRR (-68.0% to -0.3%), CH<sub>4</sub> (-85.5% to -0.1%) and N<sub>2</sub>O (0% to 364%) across climatic zones, reflecting complex interactions between environmental factors and management strategies (Bo et al., 2022). Process-based models are powerful tools for predicting and managing the complicated interactions in responses to water management, given their strength in simulating crop growth, water dynamics, and soil biogeochemical processes under diverse genotype × environment × management conditions (Tian et al., 2021; Chen et al., 2022; Yan et al., 2024). Despite with several relevant studies at site-scales, extrapolation of optimized water management schemes from limited sites to the broader rice growing regions is hindered by the diverse climate, soil, crop variety, field management, etc. (Yan et al., 2024; Liang et al., 2021). Region-specific simulations of the food-water-climate nexus are thus urgently needed to identify tailored solutions. Nevertheless, current models face challenges in accurately predicting yield responses to various water management practices and adequately reproducing the spatial heterogeneity of these responses.

Despite extensive experimental research to understand critical physiological effects underlying yield responses, these processes have not been fully represented in models, especially the compensation mechanisms. Compared to continuous flooding, imposing moderate water deficit and then rewatering the field could increase both effective leaf area and net photosynthetic rate upon re-irrigation to enhance photosynthesis for biomass production (Yang and Zhang, 2010). In addition, harvest index could increase due to enhanced remobilization of assimilates and accelerated grain filling rate (Zhang et al., 2008). However, prevailing models (for example, ORYZA, DSSAT, APSIM, WHCNS) primarily focus on the negative impacts of water deficit (i.e., reduced photosynthesis or leaf rolling), while neglecting or indirectly simulating crop adaptation processes (e.g., enhanced root growth and water uptake in deeper soil layers) (Bouman et al., 2001; Li et al., 2017; Liang et al., 2021; Tsuji et al., 1998). As a

99 consequence, yield sensitivities to water management could be overestimated, as  
100 evidenced by evaluations of the ORYZA (v3) model (Xu et al., 2018). Moreover,  
101 physiological processes respond differently to water availability at different growth  
102 stages, while crop models generally use constant water effect coefficient throughout the  
103 rice growing season (Ishfaq et al., 2020). These imply model deficiencies in predicting  
104 yield response to water management, although no assessment across large scales exists.

105  
106 Accurate model parameters are essential for reproducing spatial heterogeneity of yield,  
107 IRR, and GHGs. Previous studies usually used either the same parameters at different  
108 pixels, calibrated against all observations, or the spatial proximity principle to  
109 extrapolate model parameters for regional simulations, as a result of lacking enough  
110 observations (Zhang et al., 2024; Zhang et al., 2016). However, critical model  
111 parameters varied considerably when calibrated under different environmental and  
112 management conditions, reflecting important impact of these factors on underlying  
113 physiological and biogeochemical processes (Tan et al., 2021). As a consequence,  
114 traditional model parameterization approaches are unlikely to capture variability of  
115 yield, IRR, and GHGs due to their neglect of the environmental and management-  
116 related impacts (Song et al., 2023; Zhang et al., 2023). Besides, previous studies only  
117 evaluated simplified irrigation protocols (i.e., once drainage at midseason or alternative  
118 wetting and drying with constant threshold across the growing season) or only set bi-  
119 objectives as optimization targets (Tian et al., 2021; Chen et al., 2022), which likely  
120 underestimated the regulation potentials. Therefore, an integrated framework composed  
121 of a reliable modelling platform, broader water management schemes and multi-  
122 objective optimization targets are required for sustainable water management  
123 optimization.

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125 To address these challenges, this study proposed an advancing framework that  
126 integrated a process-based soil-crop model (Soil Water Heat Carbon Nitrogen Simulator,  
127 WHCNS) with key physiological effects, a novel model upscaling method, and the a  
128 NSGA-II multi-objective optimization algorithm (Non-dominated Sorting Genetic  
129 Algorithm II, NSGA-II) at a parallel computing platform (see Fig.1 for workflow). This  
130 study focused on rice yield (Yield), irrigation water use (IRR), methane (CH<sub>4</sub>), and  
131 nitrous oxide emissions (N<sub>2</sub>O) of irrigated rice fields. First, three physiological effects  
132 were quantified and embedded into WHCNS to enhance the prediction of yield  
133 responses. Regionalized model parameters were then derived by developing parameter  
134 transfer functions for regional simulations. The model's ability to reproduce the  
135 variations in the food-water-climate nexus was extensively validated against field  
136 observations. Multi-objective optimization was conducted using the NSGA-II  
137 algorithm to investigate tradeoffs within the food-water-climate nexus and assess the  
138 regulation potentials of water management optimization. This framework was applied  
139 to China's rice cropping system as an example, considering its position as the world's  
140 largest rice producer and the ongoing conflicts between production demand, water  
141 scarcity, and greenhouse gas emissions. This study aims to provide a valuable  
142 framework for predicting and regulating rice's food-water-climate nexus towards

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143 sustainable water management.

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## 145 **2 Data and Methods**

### 146 **2.1 WHCNS model and input data**

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148 The soil Water Heat Carbon Nitrogen Simulator (WHCNS) model was improved and  
149 incorporated into the advancing framework in this study to simulate rice yield, irrigation  
150 water use (IRR), methane (CH<sub>4</sub>), and nitrous oxide (N<sub>2</sub>O) emissions of irrigated rice  
151 fields at each pixel. The WHCNS model is a process-based agroecosystem model that  
152 runs at a daily time step and comprises six major components: surface ponding water  
153 dynamic, soil water movements, soil heat transfer, soil N transformation and transport,  
154 soil organic turnover, and crop growth. Detailed model descriptions can be found in  
155 (Liang et al., 2022; Liang et al., 2023; Liang et al., 2021). This model was chosen for  
156 several considerations: (i) the model directly outputs all four target variables  
157 simultaneously. This avoids biogeochemical models relying on crop models for detailed  
158 physiological parameters to simulate yield and calculating IRR externally to obtain all  
159 four targets as previously done (Tian et al., 2021; Yan et al., 2024), (ii) the model has  
160 been proven to simulate frequent dry-wet cycles effect reasonably well in China rice  
161 fields, due to simulating water and nitrogen dynamics in surfacing ponding water layer  
162 that is specific for rice fields (Liang et al., 2021), (iii) the model is executable at both  
163 site and regional scales with high efficiency and performs well in capturing spatial  
164 variation in key processes (Liang et al., 2023), (iv) the model has a very flexible  
165 irrigation setup, which allows for the precise control of paddy field water surface levels  
166 by setting the minimum and maximum irrigation thresholds. It also enables calculating  
167 water usage for paddy field irrigation under various water management scenarios (Jiang  
168 et al., 2021). The model is particularly suitable for simulating the regional food-water-  
169 climate nexus of rice fields.

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171 This study ran the model at both site and regional scales (0.5-degree spatial resolution).  
172 Model input data includes daily meteorological variables, soil properties by depth, and  
173 management variables related to planting, fertilization, and irrigation (Table S1). For  
174 site-scale simulations, these variables were obtained from experimental studies, if  
175 unreported, were extracted from spatial datasets according to geographical locations.  
176 All spatial datasets were all resampled to 0.5-degree spatial resolution for regional  
177 simulations. (1) Meteorological variables, including daily mean, maximum and  
178 minimum air temperature, wind speed, precipitation, humidity, and downward solar  
179 radiation, were obtained from the fifth generation ECMWF reanalysis (ERA5) at 0.25-  
180 degree resolution (Hersbach et al., 2018). (2) Soil data including bulk density, clay  
181 contents, and soil hydraulic properties (i.e., saturated water content, field water capacity,  
182 wilting point, saturated hydraulic conductivity) at soil depths of 5, 15, 30, 60, 100, and  
183 200 cm was obtained from SoilGrids (10 km) (Han et al., 2015). (3) The planting and  
184 harvest dates were obtained from the crop calendar data of Global Gridded Crop Model  
185 Intercomparisons (GGCMI) Phase 3 (Jägermeyr et al., 2021). (4) Fertilization practices  
186 were conducted by the auto-fertilization component of the WHCNS model, assuming

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187 no nitrogen stress (Liang et al., 2023). (5) Irrigation practices are defined by three  
188 variables at daily step, including upper threshold ( $U_{IRR}$ ), lower threshold ( $L_{IRR}$ , with a  
189 positive value representing field water level and a negative value representing soil water  
190 potential at 15 cm below the soil surface) and maximum allowable field water level  
191 after rainfall ( $H_p$ , also refers to as bund height). Since there is no spatially explicit  
192 information about realistic water management schemes, daily irrigation thresholds were  
193 set following Chen et al. (2022) for regional simulations. The model simulates field  
194 water level of surface ponding layer and soil water potential of stratified layers at daily  
195 step. Irrigation would be triggered whenever field water level ( $L_{IRR} > 0$ ) or soil water  
196 potential at 15 cm below the soil surface ( $L_{IRR} < 0$ ) reach the predetermined  $L_{IRR}$ .  
197 Irrigation demand is then calculated as the differences between  $L_{IRR}$  and  $U_{IRR}$ .

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## 200 2.2 Compilation of experimental observations

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202 Extensive literature reviews were conducted to collect experimental observations for  
203 model improvement and parameters calibration. Relevant studies should meet the  
204 following criteria: (1) only field experiments covering an entire growing season were  
205 included, while pot and laboratory experiments under controlled environmental  
206 conditions were excluded, (2) the control and treatments only differed concerning water  
207 management with continuous flooding (CF) as control and non-continuous flooding  
208 irrigation (NCF) as treatment, but not concerning other agronomic practices (e.g.,  
209 cropping intensity, fertilizer management, and tillage). This was to isolate water  
210 management effects while avoiding confounding effects of other factors, (3) upper and  
211 lower irrigation thresholds were explicitly reported, and lower thresholds were  
212 indicated by soil water potential measured at the soil depth of 15-20 cm. Observations  
213 based on soil water potential at the other soil depth or the other soil-water indicators  
214 (e.g., soil water contents) were excluded, (4) at least one of target variables were  
215 observed, including rice yield (*Yield*), irrigation water use (*IRR*), methane emissions  
216 ( $CH_4$ ), nitrous oxide emissions ( $N_2O$ ), leaf area index (*LAI*), net photosynthetic rate  
217 (*Pn*), and harvest index (*HI*). For *LAI* and *Pn*, the growth stages of observations (i.e.,  
218 tillering, booting, heading, and ripening stage) were recorded to account for growth  
219 stage-dependent effects. As a result, we collected observations of 119 experiments from  
220 37 studies covering 29-28 sites in 6 countries (i.e., China, India, Philippines, Japan,  
221 Bangladesh, and Peru) (Fig. S1). These observations were split into two datasets  
222 according to target variables. The first dataset including *Yield*, *IRR*,  $CH_4$ , or  $N_2O$   
223 observations was used for calibration of model parameters. The second dataset of *LAI*,  
224 *Pn*, or *HI* observations was used to quantify water management effects on physiological  
225 processes for model improvement (Section 2.3).

226

227 For each paired observation under the control and treatment, the effects of non-  
228 continuous flooding irrigation were calculated as the ratio of observations under  
229 treatment to that under control (Equation 1). This yielded 251 records for  $R^{Yield}$ , 235 for  
230  $R^{IRR}$ , 37 for  $R^{CH_4}$ , 14 for  $R^{N_2O}$ , 561 for  $R^{LAI}$  (including 61 from tillering stage, 159 from

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231 booting stage, 202 from heading stage and 139 from ripening stage), 84 for  $R^{Pn}$   
 232 (including 42 from tillering stage, and 42 from filling stage), and 351 for  $R^{HI}$ .  
 233

$$234 \quad R^X = \frac{X_{NCF}}{X_{CF}} \quad (1)$$

235 where  $R^X$  represents non-continuous flooding effects ( $NCF$ ) on target variables  $X$   
 236 (including  $Yield$ ,  $IRR$ ,  $CH_4$ ,  $N_2O$ ,  $LAI$ ,  $Pn$ , and  $HI$ ),  $X_{NCF}$  and  $X_{CF}$  represent variable  
 237 values under non-continuous flooding ( $NCF$ ) and continuous-flooding irrigation ( $CF$ ),  
 238 respectively. Relative changes of target variables were calculated as  $(R^X-1) \times 100$  for  
 239 interpretation and representation (e.g.,  $\Delta Yield$ ,  $\Delta IRR$ ,  $\Delta CH_4$ ,  $\Delta N_2O$ ).  
 240

241 For each paired observation, four categories of information were also collected. First,  
 242 climatic variables included mean daily air temperature ( $T$ ), precipitation ( $P$ ), and crop  
 243 evapotranspiration ( $PET_c$ ) during growing season. The difference between  $P$  and  $PET_c$   
 244 was further calculated to indicate climatological water availability ( $CWA$ ). Second, soil  
 245 variables included sand content, bulk density (BD), soil organic carbon ( $SOC$ ), pH, and  
 246 soil hydrological properties (e.g., saturated water content ( $SAT$ ), field water capacity  
 247 ( $FWC$ )). Third, management-related variables included nitrogen application rate and  
 248 timing, as well as lower ( $L_{AWD}$ ) and upper ( $U_{AWD}$ ) irrigation thresholds. Fourth,  
 249 experimental parameters included geographical location (latitude, longitude), dates of  
 250 seeding (also transplanting date in transplanted systems), anthesis, and harvest. These  
 251 variables were used for running WHCNS (Section 2.1) and conducting correlation  
 252 analyses (Section 3.1).  
 253

## 254 **2.3 Model improvement**

### 255 **2.3.1 Incorporation of physiological effects**

256  
 257 In the original WHCNS model, water management effects on crop growth were  
 258 simulated by calculating water stress factor based on the Feddes reduction function  
 259 (Feddes and Zaradny, 1978). Specifically, the water stress factor is calculated at daily  
 260 step as a function of soil water potential to reduce root water uptake, assuming 70 kpa  
 261 and 1500 kpa as thresholds of when root water uptake starts to decrease and approaches  
 262 0 (Equation 2-3). The calculated water stress factor was used to reduce the simulated  
 263 actual biomass production rate, which further indirectly impact produced biomass  
 264 allocated for leaf growth and yield formation (Equation 4-6).  
 265

$$266 \quad T_a = \int_{L_R} S(h, h_\phi, z) dz = T_p \int_{L_R} a_w(h, z) a_s(h_\phi, z) b(z) dz \quad (2)$$

$$cf(w) = \frac{T_a}{T_p} = \begin{cases} \frac{\int_{L_R} a_w(h,z) a_s(h_\phi, z) b(z) dz}{\omega} = \frac{\omega}{\omega} = 1 & \omega > \omega_c \\ \frac{\int_{L_R} a_w(h,z) a_s(h_\phi, z) b(z) dz}{\omega_c} = \frac{\omega}{\omega_c} < 1 & \omega \leq \omega_c \end{cases} \quad (3)$$

$$Fgc = DL \times \frac{AMAX}{K_e} \times \ln \left[ \frac{AMAX + CC}{AMAX + CC \times (-LAI \times K_e)} \right] \quad (4)$$

$$Fgass = Fgc \times \frac{30}{44} \times cf(w) \times cf(N) \quad (5)$$

$$GAA(org) = Fgass \times fr(org) \quad (6)$$

where  $T_a$  and  $T_p$  are actual and potential root water uptake ( $\text{cm d}^{-1}$ ).  $L_R$  indicates root length (cm).  $a_w(h,z)$  and  $a_s(h_\phi, z)$  are water and salt stress functions.  $b(z)$  is root distribution function.  $w_c$  is the critical threshold of volumetric soil water content  $w$  above which root water uptake is reduced in water limited layers of the root zone, but the plant compensates by uptaking more water from other layers that have sufficient available water.  $Fgc$  is daily potential dry matter production accounting for the light interception, radiation use efficiency, and the  $\text{CO}_2$  effects ( $\text{kg hm}^{-2} \text{d}^{-1}$ ).  $AMAX$  is the maximum assimilation rate accounting for temperature effect ( $\text{kg hm}^{-2} \text{h}^{-1}$ ).  $DL$ ,  $K_e$ , and  $CC$  indicate day length ( $\text{h d}^{-1}$ ), extinction coefficient (-) and actual radiation use ( $\text{kg hm}^{-2} \text{h}^{-1}$ ).  $Fgass$  is daily actual dry matter production ( $\text{kg hm}^{-2} \text{d}^{-1}$ ) accounting for water ( $cf(w)$ ) and nitrogen stress ( $cf(N)$ ).  $GAA$  indicates produced biomass allocated to organs (leaf or grains) ( $\text{kg hm}^{-2} \text{d}^{-1}$ ) with the fraction of  $fr(org)$ .

To modify the WHCNS, NCF effects on leaf expansion, photosynthesis rate, and assimilate partition were quantified based on experimental observations and incorporated into WHCNS (Fig. S1S2). To do so, mean values of observed effects were first calculated by experimental gradient of soil water potential (SWP, negative values) and growth stages (RDS, 0-1) (Table S1S2-S3S4). RDS corresponds to planting, tillering, booting, heading, filling, and maturity stages was quantified as 0, 0.20, 0.40, 0.55, 0.75, and 1. Effects at other levels of SWP and RDS were then estimated by bilinear interpolation (i.e.,  $F^{LAI}(SWP, RDS)$ ,  $F^{Pn}(SWP, RDS)$ ,  $F^{HI}(SWP)$ ). Three functions were thus developed involving three new genetic parameters to account for differences in cultivar sensitivities ( $P^{LAI}$ ,  $P^{Pn}$ ,  $P^{HI}$ , Equations 7-9). The three functions were added to the origin crop growth module to modify simulations of leaf area index, net photosynthesis rate and biomass allocated into grains (Equation 10-12, Fig. 2a).

$$R^{LAI}(SWP, RDS) = 1 + \left[ \left( F^{LAI}(SWP, RDS) \right) - 1 \right] \times P^{LAI} \quad (7)$$

$$R^{Pn}(SWP, RDS) = 1 + \left[ \left( F^{Pn}(SWP, RDS) \right) - 1 \right] \times P^{Pn} \quad (8)$$

$$R^{HI}(SWP) = 1 + \left[ \left( F^{HI}(SWP) \right) - 1 \right] \times P^{HI} \quad (9)$$

$$LAI' = GAA(leaf) \times SLA \times R^{LAI} \quad (10)$$

$$AMAX' = AMAX \times R^{Pn} \quad (11)$$

$$GAA(grains)' = Fgass \times fr(grains) \times R^{HI} \quad (12)$$

where  $R^{LAI}$ ,  $R^{Pn}$ ,  $R^{HI}$  represent NCF effects on leaf area index, net photosynthetic rate and harvest index, respectively.  $SWP$  represents soil water potential at 15-20 cm soil depth.  $RDS$  represents relative development stages (0-1).  $P^{LAI}$ ,  $P^{Pn}$ , and  $P^{HI}$  are genetic parameters indicating cultivar sensitivities to irrigation regulation that were calibrated based on observations (Section 2.4).  $LAI$  and  $SLA$  are leaf area index ( $m^2 m^{-2}$ ) and specific leaf area ( $m^2 kg^{-1}$ ).  $LAI'$ ,  $AMAX'$  and  $GAA(grains)'$  denote simulations of the modified model. It is worth noting that the three functions can be flexibly coupled to the other process-based crop models to modify the simulation of leaf area growth, biomass production, and allocation processes. The genetic parameters are needed to be recalibrated against observed yield responses considering different model structures.

### 2.3.2 Contribution analysis

Scenario simulations were conducted to isolate contributions of the three physiological effects on yield changes ( $\Delta Yield$ ) (Table S4S5). Four scenarios were simulated by considering all the three effects (S1) and omitting one of the three effects at a time (S2-S4). For each scenario, the model was run under CF and NCF conditions respectively to calculate  $\Delta Yield$ . The differences in the simulated  $\Delta Yield$  between S1 and S2-S4 represent yield changes induced by changes in leaf expansion, photosynthesis rate and assimilate partition, respectively (i.e.,  $\Delta Yield^{LAI}$ ,  $\Delta Yield^{Pn}$ ,  $\Delta Yield^{HI}$ ). Relative contribution of each process was calculated as the ratio of the absolute yield change induced by the process to the sum of absolute yield change induced by the three processes (Equation 13).

$$CON^p = \frac{|\Delta Yield^p|}{\sum_{p=1}^3 |\Delta Yield^p|} \times 100 \quad (13)$$

where  $p$  represents the three new physiological processes (i.e.,  $p = 1, 2, 3$ ),  $CON^p$  indicates relative contribution of the process  $p$  to  $\Delta Yield$ ,  $\Delta Yield^p$  is yield changes induced by the process  $p$ .

## 335 2.4 Parameters regionalization

336

337 Spatially explicit model parameters are critical for reasonably reproducing spatial  
338 variabilities of target variables. In this study, seven key model parameters were selected  
339 and mapped at 0.5-degree spatial resolution due to their high influence on target  
340 variables, including accumulated temperature for crop maturity (*Cumtemp*), minimum  
341 assimilation rates (*AMIN*), the maximum CH<sub>4</sub> production rate per soil weight at 30 °C  
342 (*MPmax*), maximum portion of denitrification to N<sub>2</sub>O production ( $f_{N2O\_d}$ ) and the three  
343 new genetic parameters ( $P^{LAI}$ ,  $P^{Pn}$ ,  $P^{HI}$ ). These parameters were first finely calibrated at  
344 site-scales (Section 2.4.1) and then upscaled to regional scales (Section 2.4.2). To  
345 capture spatial variabilities of NCF effects, different parameters were used under CF  
346 and NCF conditions, except for genetic parameters. This was consistent with a previous  
347 modelling study, aiming to indicate different potentials of methane production and  
348 denitrification under different water management regimes (Song et al., 2023).

349

### 350 2.4.1 Calibration of site-scale parameters

351

352 Under CF conditions, the parameter *Cumtemp* was first determined by cultivar as the  
353 minimum cumulative daily temperature higher than 10°C (base temperature for rice  
354 growth) across all experiments using the cultivar. Then *AMIN*, *MPmax* and  $f_{N2O\_d}$  were  
355 calibrated to achieve the best fit of predicted target variables with observations under  
356 continuous flooding conditions (i.e., experimental control). Under NCF conditions,  
357 *Cumtemp* and *AMIN* were the same with that calibrated from CF conditions. The other  
358 parameters (*MPmax*,  $f_{N2O\_d}$ ,  $P^{LAI}$ ,  $P^{Pn}$  and  $P^{HI}$ ) were then calibrated by minimizing the  
359 sum of simulated squared residuals under non-continuous flooding conditions (Table  
360 S5S6). To obtain more accurate parameter estimates, the advanced parameter  
361 estimation algorithm (PEST) was used (Doherty, 2010). As a result, 51 groups of  
362 genetic parameters (*Cumtemp*, *AMIN*,  $P^{LAI}$ ,  $P^{Pn}$  and  $P^{HI}$ ), 56 parameter values of  
363 *MPmax* (19 for control and 37 for treatment) and 24 parameter values of  $f_{N2O\_d}$  (10 for  
364 control and 14 for treatment) were calibrated.

365

### 366 2.4.2 Parameters upscaling

367

368 To upscale genetic parameters (*AMIN*, *Cumtemp*,  $P^{LAI}$ ,  $P^{Pn}$ ,  $P^{HI}$ ) calibrated at site  
369 scales to regional scales, the rice cultivar for each grid was first determined. Then, the  
370 calibrated genetic parameters of the cultivar were used to create the grid. Since the  
371 spatial distribution of rice cultivar is unknown, cultivar of each grid cell was  
372 determined as follows. First, cultivars with *Cumtemp* lower than the effective  
373 accumulative temperature requirement of the grid were identified. This ensures the  
374 cultivar could reach maturity under the grid cell's temperature conditions. The grid's  
375 temperature requirement was calculated as *Cumtemp* during rice growing periods  
376 specified by the crop calendar data of GGCM Phase 3 (Jägermeyr et al., 2021).  
377 Subsequently, cultivars with *AMIN* that closely match the baseline *AMIN* of the grid  
378 cell were selected. The baseline *AMIN* was estimated using PEST to achieve the best

379 fit of yield simulation with the records in county-scale statistical yearbooks of China  
 380 (downscaled to 0.5-deg spatial resolution). These procedures were designed to ensure  
 381 that yield simulations were aligned with cultivar's genetic potential and spatially  
 382 consistent with observations.

383  
 384 To upscale parameters  $MP_{max}$  and  $f_{N_2O\_d}$ , two parameter transfer functions (PTFs)  
 385 were developed. Dependent variables were the ratio of site-calibrated parameters  
 386 under treatment to that under control (i.e.,  $R^{MP_{max}}$  and  $R^{f_{N_2O\_d}}$ ) (Equation 16-17).  
 387 Independent variables were determined as field water capacity ( $FWC$ ) for  $R^{MP_{max}}$  and  
 388 bulk density ( $BD$ ) for  $R^{f_{N_2O\_d}}$ , due to their higher correlations with dependent  
 389 variables. The function forms were determined as the form with the highest  $R^2$ . As a  
 390 result, the relationship between field water capacity and  $R^{MP_{max}}$  was best fitted by an  
 391 exponential function ( $R^2 = 0.62$ ,  $p < 0.001$ ), and the relationship between bulk density  
 392 and  $R^{f_{N_2O\_d}}$  was best fitted by a quadratic function ( $R^2 = 0.91$ ,  $p < 0.001$ ) (Fig. S4S5).  
 393 The importance of soil properties in regulating spatial heterogeneity of denitrification  
 394 potentials aligns with previous studies (Tang et al., 2024). Parameters of the PTFs  
 395 were calibrated using the least square method (Equation 16-17). With the calibrated  
 396 PTFs, the ratio of parameters under NCF relative to CF ( $R^{MP_{max}}$  and  $R^{f_{N_2O\_d}}$ ) for each  
 397 grid could be predicted by combining spatial dataset of  $FWC$  and  $BD$ . Then gridded  
 398  $MP_{max}$  and  $f_{N_2O\_d}$  for CF conditions ( $MP_{max}^{CF}$  and  $f_{N_2O\_d}^{CF}$ ) were estimated using PEST  
 399 targeting  $CH_4$  from the EDYGA v8.0 dataset (Crippa et al., 2024) and  $N_2O$  emissions  
 400 estimated by Cui et al. (2024) (Fig. S3S4). These parameters were estimated for 2013  
 401 and 2015 and subsequently validated for 2014 and 2016 to assess their ability to  
 402 reproduce the spatial variability of target variables (Fig. S2S3). Finally,  $MP_{max}$  and  
 403  $f_{N_2O\_d}$  for NCF conditions were calculated by multiplying  $MP_{max}^{CF}$  and  $f_{N_2O\_d}^{CF}$  with  
 404 the predicted ratio ( $R^{MP_{max}}$  and  $R^{f_{N_2O\_d}}$ ).

405  
 406

$$407 \quad R^{MP_{max}} = MP_{max}^{NCF} / MP_{max}^{CF} = 986 \times e^{-26 \times FWC} \quad (16)$$

$$408 \quad R^{f_{N_2O\_d}} = f_{N_2O\_d}^{NCF} / f_{N_2O\_d}^{CF} = 268 \times BD^2 + 789 \times BD + 581 \quad (17)$$

409

410 Where  $R^{MP_{max}}$  and  $R^{f_{N_2O\_d}}$  represent the ratio of parameter  $MP_{max}$  and  $f_{N_2O\_d}$   
 411 calibrated under non-continuous flooding (treatment) to that under continuous  
 412 flooding (control).  $FWC$  and  $BD$  represent field water capacity ( $cm^3 cm^{-3}$ ) and soil  
 413 bulk density ( $g cm^{-3}$ ) obtained from SoilGrids (10 km) (Han et al., 2015).

414

415 To prove the efficacy of the PTFs, two other parameter upscaling approaches were also  
 416 used for comparison, including the mean parameters approach and the spatial proximity  
 417 approach. These approaches were widely used in previous modelling studies to derive  
 418 regional parameters and conduct regional simulations (Zhang et al., 2024). To adopt the  
 419 mean parameter approach, mean value of the site-calibrated  $MP_{max}$  and  $f_{N_2O\_d}$  (Section  
 420 2.4.1) were calculated respectively for CF and NCF conditions, and then the two



465 solution under the four single-objective scenarios, the largest regulation potentials to  
 466 increase yield and reduce IRR, CH<sub>4</sub>, and N<sub>2</sub>O emissions were assessed. For comparison,  
 467 the scenario simulations and optimization were also conducted using the origin  
 468 WHCNS model (Fig. 5).

469  
 470 The multi-objective optimization was conducted by combining the improved WHCNS  
 471 model and the NSGA-II algorithm (Deb et al., 2002). First, a set of 100 parental  
 472 populations was initialized with random solutions. Each population includes 1993  
 473 individuals, corresponding to 1993 grid cells of irrigated rice areas. Second, the  
 474 objective functions were computed with each solution by executing the WHCNS model  
 475 (Equation 18). Third, the performance of each population was evaluated by ranking the  
 476 fitness of its objective functions. Fitness is a measure of how well a solution performs  
 477 and is calculated based on the non-dominated sorting rank. Then, a new generation was  
 478 generated through selection, crossover, and mutation based on fitness. Finally, Pareto  
 479 fronts were generated after 100 generations had been evaluated (that is 10000  
 480 populations).

481

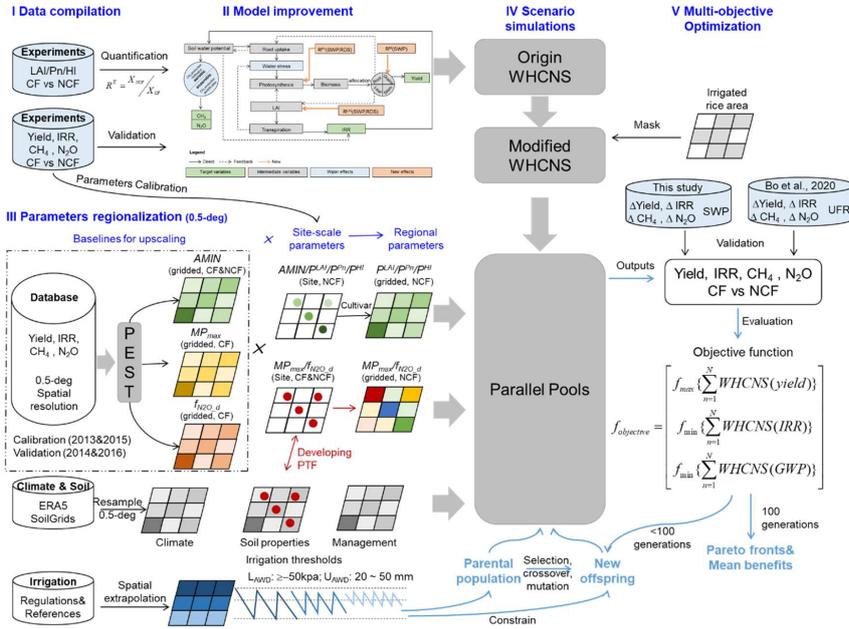
$$f_{objective} = \begin{bmatrix} f_{max} \left\{ \sum_{n=1}^N WHCNS(yield) \right\} \\ f_{min} \left\{ \sum_{n=1}^N WHCNS(IRR) \right\} \\ f_{min} \left\{ \sum_{n=1}^N WHCNS(GWP) \right\} \end{bmatrix} \quad (18)$$

$$WHCNS(GWP) = 27.2 \times WHCNS(CH_4) + 273 \times WHCNS(N_2O) \quad (19)$$

484 where  $f_{objective}(yield, IRR, GWP)$  denotes the collection of objective functions,  $f_{max}$   
 485 denotes the objective that needs to be maximized (e.g., rice yield), and  $f_{min}$  denotes the  
 486 objective that needs to be minimized (e.g., IRR, GWP). GWP is the integrated global  
 487 warming potential of combined emissions of CH<sub>4</sub> and N<sub>2</sub>O emissions and is  
 488 calculated based on WHCNS simulations (Equation 19) (Forster et al., 2021). It  
 489 should be noted that this study set equal weight for each target variable to evaluate the  
 490 fitness of each solution. Decision-makers can simply set the weight values of different  
 491 objectives according to their preferences, or adopt advanced multi-objective criteria  
 492 decision-making methods such as the efficiency coefficient method (Guo et al., 2021).  
 493 The regulation potentials of multiple-objective optimization were calculated as the  
 494 averaged NCF effects ( $\Delta Yield$ ,  $\Delta IRR$ ,  $\Delta CH_4$ ,  $\Delta N_2O$ ,  $\Delta GWP$ ) of all non-dominated  
 495 solutions. The potentials were further compared with that from single-objective  
 496 optimizations to investigate tradeoffs between target variables (Fig. 6).  
 497

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499 **Figure 1 Research framework of this study.** The framework mainly combines *data*  
500 *compilation, model improvement, parameter regionalization, scenario simulations, and*  
501 *multi-objective optimization.* The framework can be flexibly adapted with alternative  
502 irrigation scenarios, optimization objectives, and optimization algorithms in other  
503 modelling studies. *LAI, Pn,* and *HI* represent leaf area index, net photosynthetic rate,  
504 and harvest index. *AMIN, MPmax, fN2O\_d, PLAI, Pp,* and *PHi* are model parameters  
505 calibrated and mapped in this study (Section 2.4). *CF* and *NCF* represent continuous  
506 flooding and non-continuous flooding irrigation. *SWP* and *UFR* represent soil water  
507 potential and the ratio of unflooded days to total rice growing days, indicating different  
508 irrigation schemes. See the *Appendix* for detailed descriptions of parameters and  
509 variables.

510

### 511 3 Results and discussion

#### 512 3.1 Performance of model improvement

513

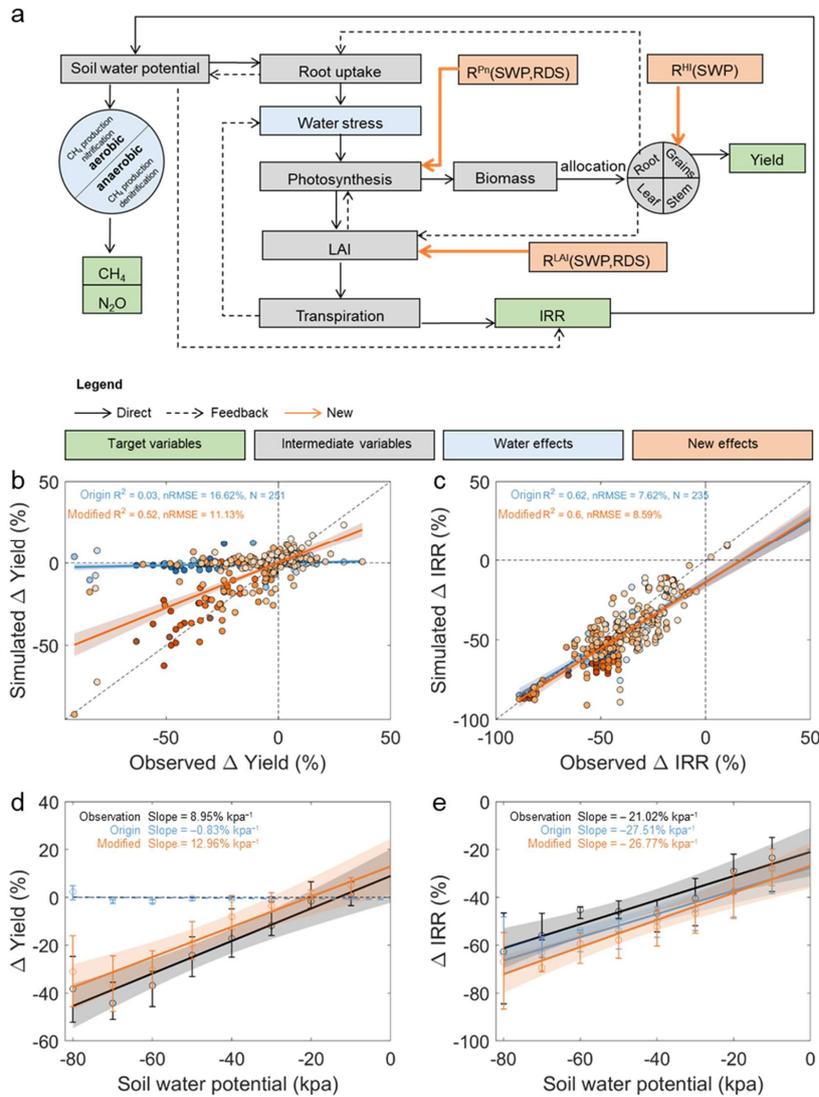
514 The origin WHCNS model was first evaluated in reproducing variabilities of rice yield  
515 and irrigation water use under various irrigation schemes. For rice yield, model  
516 performance is satisfying when mixing observations under continuous flooding (CF,  
517 experimental control) and non-continuous flooding (NCF, experimental treatments)  
518 irrigation schemes together ( $R^2 = 0.41$ , normalized root mean square error  $nRMSE =$   
519  $11\%$ ) (Fig. S5S6). In particular, with fine-tuned crop genetic parameters (i.e., *Cumtemp*  
520 and *AMIN*), the origin model performed well under CF condition ( $R^2 = 0.74$ ,  $nRMSE =$   
521  $13\%$ ), while had worse performance under NCF condition ( $R^2 = 0.22$ ,  $nRMSE = 13\%$ )

522 (Fig. S5S6). As a consequence, the origin model failed to reproduce variations in  
523 observed yield changes ( $\Delta\text{Yield}$ ) ( $R^2 = 0.03$ ,  $nRMSE = 17\%$ ) (Fig. 2b). More importantly,  
524 the simulations could not reproduce  $\Delta\text{Yield}$  sensitivities to soil water potentials  
525 presented in field experiments (Fig. 2d). In contrast to yield, model performance in  
526 simulating irrigation water use responses ( $\Delta\text{IRR}$ ) variabilities and its sensitivities to soil  
527 water potentials was acceptable (Fig. 2c and 2e). These results highlight the primary  
528 modelling deficiency in simulating  $\Delta\text{Yield}$ . Given the satisfying model performance in  
529 simulating yield under CF and  $\Delta\text{IRR}$ , the underperformance is likely due to lacking  
530 critical physiological processes responsible for yield responses to NCF rather than  
531 uncertainties of crop parameters.

532  
533 After incorporating the three functions of NCF effects and fine calibration of genetic  
534 parameters (Section 2.3, Fig. 2a), the model performance was substantially improved.  
535 The explained variabilities of  $\Delta\text{Yield}$  increased from 3% to 52% and  $nRMSE$  decreased  
536 from 17 % to 11% (Fig. 2b). The observed  $\Delta\text{Yield}$  sensitivities to soil water potential  
537 ( $9\% \text{ kpa}^{-1}$ ,  $P < 0.001$ ) could be reasonably reproduced by the modified model ( $13\%$   
538  $\text{kpa}^{-1}$ ,  $P < 0.001$ ) rather than the origin mdoel ( $P > 0.05$ ) (Fig. 2d). The cultivar  
539 differences of yield responses could also be simulated ( $R = 0.67$ ) (Fig. S6S7). Across  
540 the three processes, leaf area growth ( $\Delta\text{Yield}^{LA}$ ) was primarily responsible for yield  
541 losses, while net photosynthetic rate ( $\Delta\text{Yield}^{Pn}$ ) and biomass translocation ( $\Delta\text{Yield}^{H}$ )  
542 contributed to yield increases (Section 2.3.2, Fig. S7S8). The positive contributions are  
543 larger in warmer and more humid areas, and in acidic soils with larger field water  
544 holding capacity and higher SOC. These findings conform with empirical relationships  
545 between  $\Delta\text{Yield}$  and environmental factors reported by previous meta-analysis (Carrizo  
546 et al., 2017). These results prove efficacy of the modified model to predict and regulate  
547  $\Delta\text{Yield}$  under diverse irrigation schemes and environmental conditions.

548  
549 ~~Besides being coupled to WHCNS as an integrated system, the new functions also~~  
550 ~~contribute to advancing related modelling studies by directly involving positive~~  
551 ~~physiological effects and considering stage-dependent response sensitivities (Li et al.,~~  
552 ~~2017). By contrast, most prevailing crop models only account for negative effects of~~  
553 ~~soil drying and reduced transpiration, while does not incorporating direct compensation~~  
554 ~~effects (such as increased photosynthesis rate upon rewatering). Moreover, constant~~  
555 ~~stress sensitivity parameters were generally used for all growth stages (such as ORYZA~~  
556 ~~and DSSAT) (Bouman et al., 2001; Tsuji et al., 1998). These models could flexibly~~  
557 ~~incorporate the three new functions and recalibrate the genetic parameters (i.e.,  $P^{LA}$ ,~~  
558  ~~$P^{Pn}$ , and  $P^H$ ) following the procedures of this study to improve their performance in~~  
559 ~~predicting yield responses.~~

560



561

562 **Figure 2 Model improvements by incorporating water effects on physiological**  
 563 **processes. (a)** Schematic of critical physiological effects in response to different  
 564 irrigation schemes and their representation in the WHCNS model. **(b-c)** Model  
 565 performance for simulating ΔYield **(b)** and ΔIRR **(c)** based on the origin (blue) and  
 566 modified (orange) WHCNS model. Darker colored dots indicate lower soil water  
 567 potential (unit: kpa). **(d-e)** Sensitivity of ΔYield and ΔIRR to lower irrigation threshold  
 568 of soil water potential. Black, blue, and orange colors show the results of observations  
 569 and simulations based on the origin and modified WHCNS model, respectively. Circles

570 are mean values; error bars show the 25–75% interquartile range. The lines are the  
571 linear regression lines with dashed lines indicating non-significant relationships based  
572 on two-sided t-test ( $P > 0.05$ ). The shaded areas around each line represent the 95%  
573 confidence interval.

574  
575 Besides being coupled to WHCNS as an integrated system, the new functions also  
576 contribute to advancing related modelling studies by directly involving positive  
577 physiological effects and considering stage-dependent response sensitivities (Li et al.,  
578 2017). By contrast, most prevailing crop models only account for negative effects of  
579 soil drying and reduced transpiration, while does not incorporating direct compensation  
580 effects (such as increased photosynthesis rate upon rewatering) . Moreover, constant  
581 stress sensitivity parameters were generally used for all growth stages (such as ORYZA  
582 and DSSAT) (Bouman et al., 2001; Tsuji et al., 1998). These models could flexibly  
583 incorporate the three new functions and recalibrate the genetic parameters (i.e.,  $P^{LAI}$ ,  
584  $P^{Pn}$ , and  $P^{HI}$ ) following the procedures of this study to improve their performance in  
585 predicting yield responses.

586

### 587 **3.2 Performance of regionalized parameters**

588

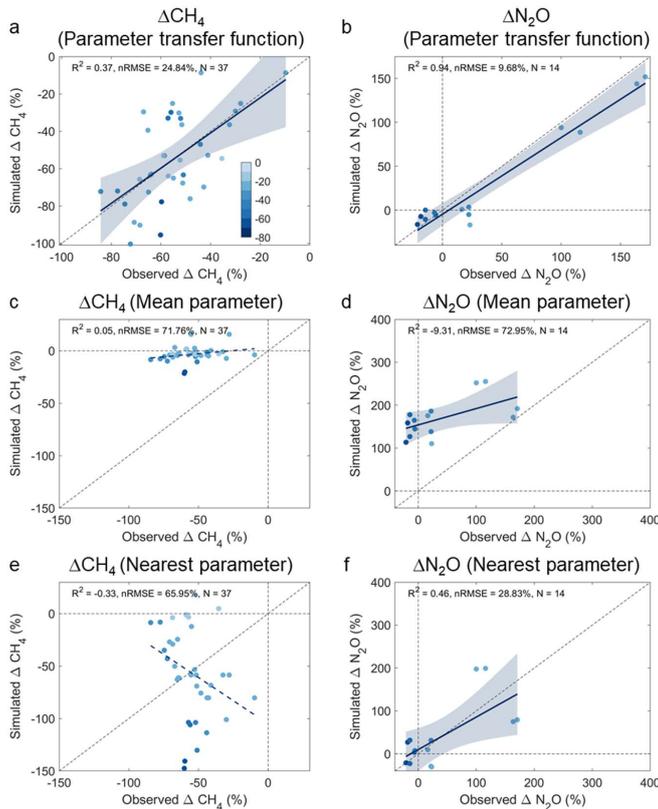
589 To simulate regional NCF effects, the model was first run respectively for CF (baseline)  
590 and NCF conditions using the parallel computing framework at a spatial resolution of  
591 0.5-deg. NCF effects were then calculated using model simulations following Equation  
592 1 (Fig.1 and Section 2.4). Using the PEST-calibrated gridded model parameters for CF  
593 (Section 2.4.1), the  $nRMSE$  between model simulations and their spatial datasets were  
594 20% to 29% for yield, ~7% for IRR, ~4% for  $CH_4$ , and 4% to 6% for  $N_2O$  during the  
595 validation period (year 2014 and 2016) (Fig.S2). It was noted that the  $nRMSE$  of rice  
596 yield was relatively larger than that of other target variables, despite being within an  
597 acceptable range (<30% for the validation periods). This could be caused by interannual  
598 cultivar changes, which was difficult to consider in large-scale simulations due to the  
599 lack of spatial distribution of rice cultivars. Overall, these results reveal a satisfying  
600 model calibration to simulate baseline values and spatial variabilities of target variables.

601

602 To reproduce observed variabilities of NCF effects on target variables, NCF effects on  
603 key model parameters ( $MP_{max}$  and  $f_{N_2O,d}$ ) were incorporated for constraining model  
604 simulations. To do so, NCF effects on model parameters were first quantified from site-  
605 scale calibrations and extrapolated to regional scale (Section 2.4). Three approaches of  
606 parameter extrapolation were tested and compared, including developing parameter  
607 transfer functions (PTFs), using mean site-calibrated parameters (mean), and using  
608 spatially nearest calibrated parameters (spatial) (Section 2.4.3). Results showed that  
609 developing PTFs performed the best to reproduce observed variabilities of  $\Delta CH_4$  and  
610  $\Delta N_2O$  (Fig. 3). Model simulations using parameters estimated by PTFs explained 37%  
611 and 94% of variations in  $\Delta CH_4$  and  $\Delta N_2O$ , with  $nRMSE$  being 25% for  $\Delta CH_4$  and 10%  
612 for  $\Delta N_2O$  (Fig. 3a-b). By contrast, simulations based on the other two approaches could  
613 hardly reproduce observed variabilities of  $\Delta CH_4$  and  $\Delta N_2O$ , with  $nRMSE$  achieving 66%

614 to 72% for  $\Delta\text{CH}_4$  and 29% to 73% for  $\Delta\text{N}_2\text{O}$  (Fig. 3c-f). These results prove the efficacy  
 615 of the developed PTFs and suggest soil variables as good predictors for spatial  
 616 extrapolation of site-calibrated parameters to simulate  $\text{CH}_4$  and  $\text{N}_2\text{O}$ . The PTFs could  
 617 also be referred by other biogeochemical models for regional simulations of  $\text{CH}_4$  and  
 618  $\text{N}_2\text{O}$  (such as the Denitrification-Decomposition model DNDC and the Dynamic Land  
 619 Ecosystem Model DLEM) (Zhang et al., 2016).  
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621  
 622 **Figure 3 Comparison of model parameter upscaling approaches.** Model  
 623 performance in simulating methane and nitrous oxide emissions changes based on  
 624 parameters derived from (a-b) parameter transfer functions (PTFs), (c-d) mean site-  
 625 calibrated parameters, and (e-f) spatially nearest parameters. The color of the dots  
 626 indicates lower irrigation thresholds of soil water potential under non-continuous  
 627 flooding irrigation (unit: kpa). The solid lines are regression lines with dashed lines  
 628 indicating non-significant relationships ( $P > 0.05$ ). Blue shading around each line  
 629 represents the 95% confidence interval.  
 630

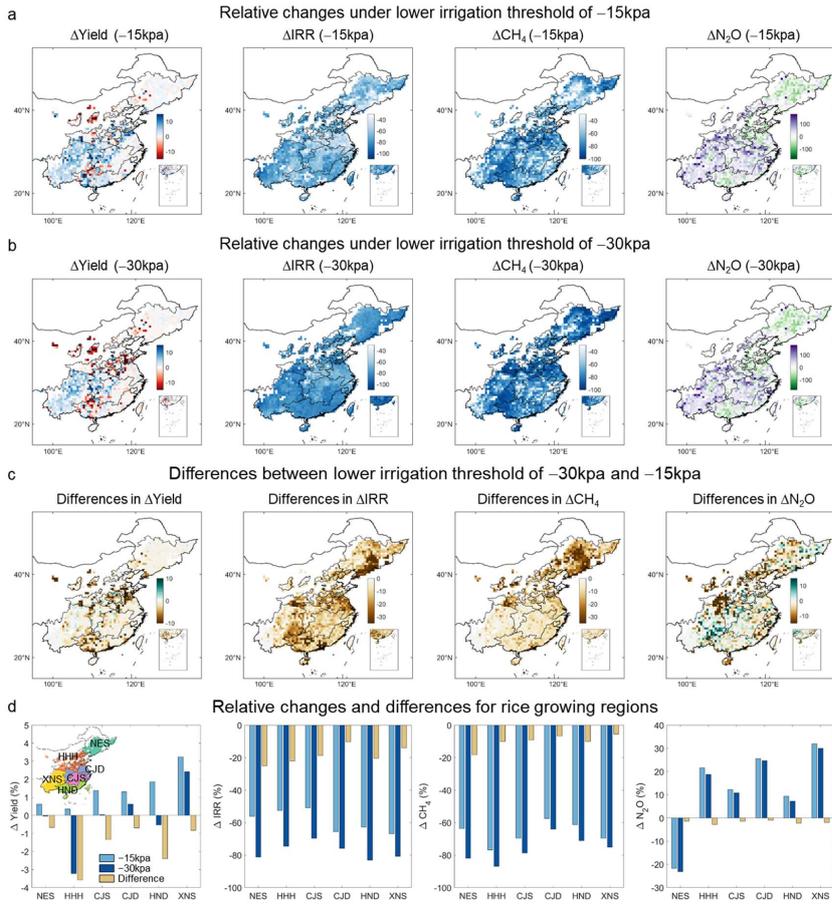
631 Considering scarce observations of NCF effects across space, it was impractical to  
 632 directly evaluate the regionalized parameters in reproducing spatial



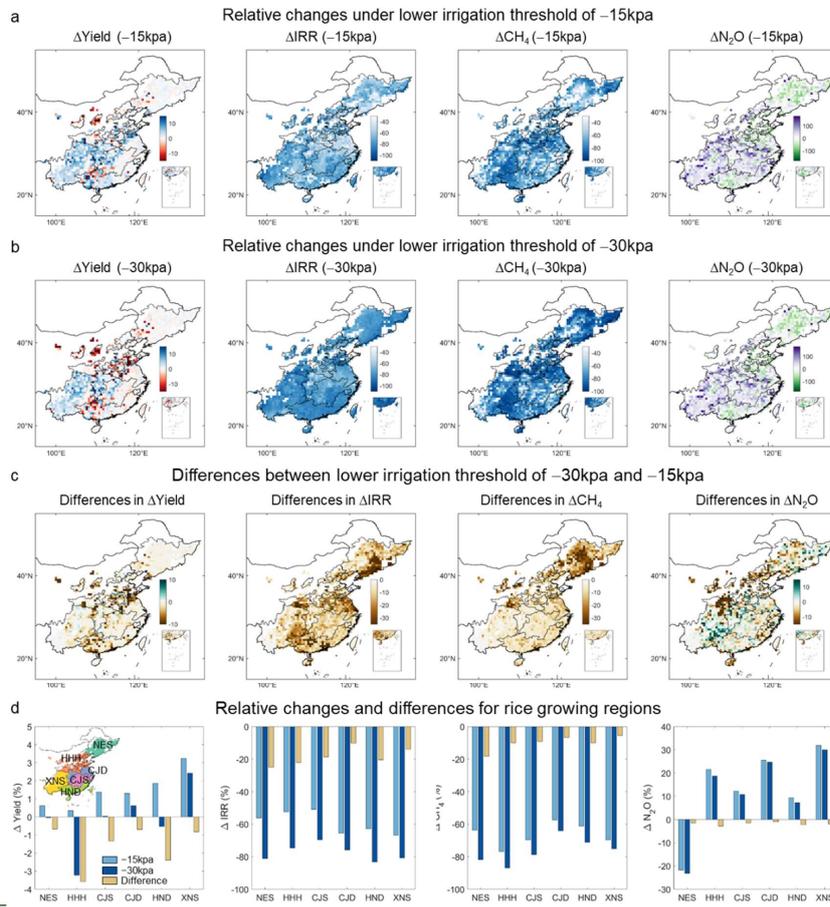
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CH<sub>4</sub> and N<sub>2</sub>O emissions were dominated by edaphic factors regardless of irrigation threshold (i.e., clay for CH<sub>4</sub> and bulk density for N<sub>2</sub>O) (Fig. 5c and d). These findings highlight the complex interplay of factors influencing regulation potentials of rice production, irrigation water use and greenhouse gas emissions through NCF adoption.

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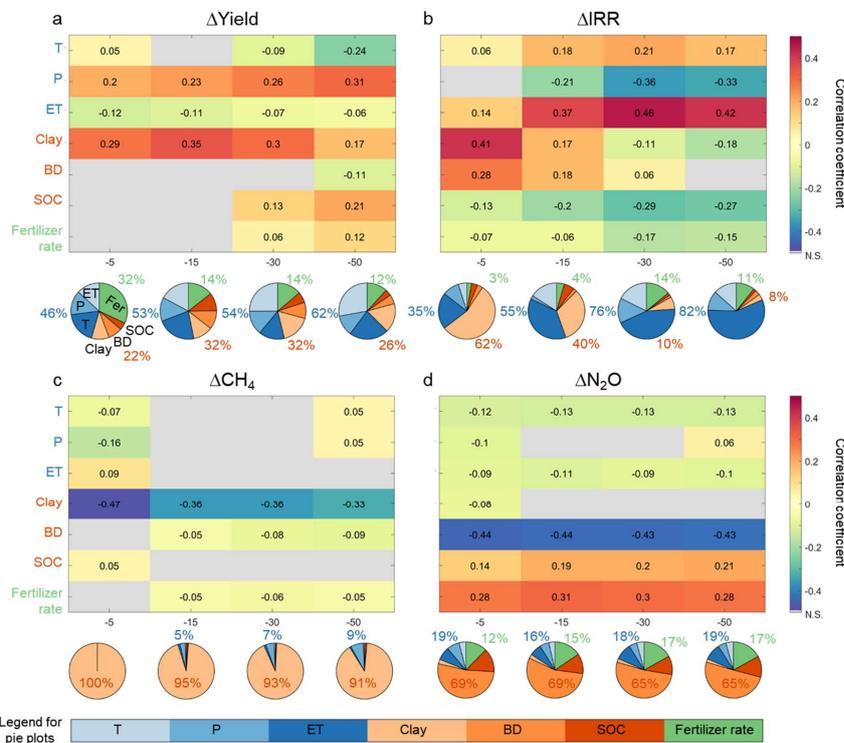
684 **Figure 4 Spatial pattern of relative changes in target variables under different**  
 685 **irrigation schemes and differences.** The four columns correspond to the four target  
 686 variables  $\Delta$ Yield,  $\Delta$ IRR,  $\Delta$ CH<sub>4</sub>, and  $\Delta$ N<sub>2</sub>O, respectively. (a) relative changes of target  
 687 variables under a lower irrigation potential of -15 kpa, (b) relative changes of target  
 688 variables under a lower irrigation potential of -30 kpa, (c) differences between (b) and  
 689 (a), (d) results for different rice growing regions. NES, HHH, CJS, CJD, HND, and  
 690 XNS indicate six rice growing areas of China, namely, Northeast Single rice,  
 691 HuangHuaiHai single rice, Yangtze River single rice, Yangtze River double Rice, South  
 692 China Double rice, and Southwest China Single rice, respectively.

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697 **Figure 5 Drivers regulating spatial variations in relative changes in yield (a), IRR**  
 698 **(b), CH<sub>4</sub> (c) and N<sub>2</sub>O (d).** The numbers and colors indicate correlation coefficients,  
 699 with gray indicating non-significant correlations (N.S., P > 0.05). The pie plots  
 700 represent the proportion of irrigated rice areas (%) for which relative changes  
 701 variation is regulated by the dominant drivers. The dominant driver is defined as the  
 702 factor with the largest absolute correlation coefficient in each grid cell, identified from  
 703 3.5°-by-3.5° moving windows. The numbers in blue, orange and green around the pie  
 704 plots denote the area proportions dominated by climate (i.e., T + P + ET), soil (i.e.,  
 705 Clay + BD + SOC) and management-related (i.e., Fertilizer rate) factors under  
 706 corresponding lower irrigation threshold. Spatial distributions of dominant drivers are  
 707 shown in Fig. S10 and S11.

708  
 709 Four single objective targets were designed to identify the largest regulation  
 710 potentials from NCF adoption, four single objective targets were designed, including  
 711 maximizing rice yield, minimizing IRR, CH<sub>4</sub> emissions, or N<sub>2</sub>O emissions (denoted as  
 712 maxYield, minIRR, minCH<sub>4</sub>, min N<sub>2</sub>O, Section 2.6). Results indicated that the largest  
 713 regulation potentials of ΔYield, ΔIRR, ΔCH<sub>4</sub> and ΔN<sub>2</sub>O were 4.6%, -61.0%, -64.2%  
 714 and -10.9%, respectively (Fig. 5a6a). These potentials could be achieved respectively

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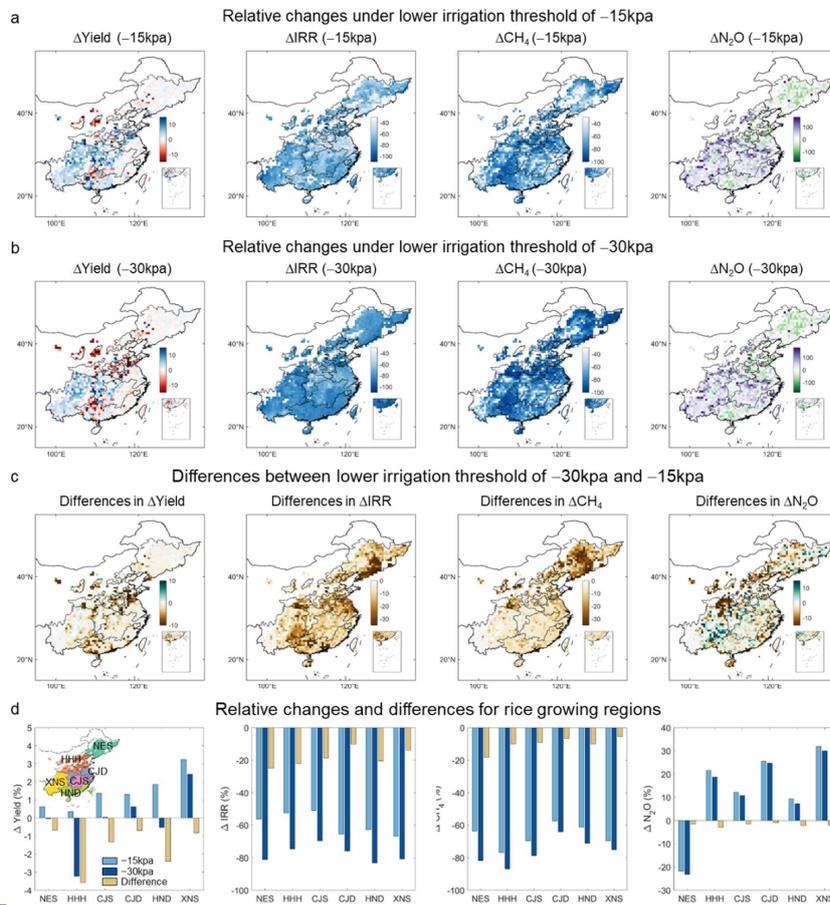
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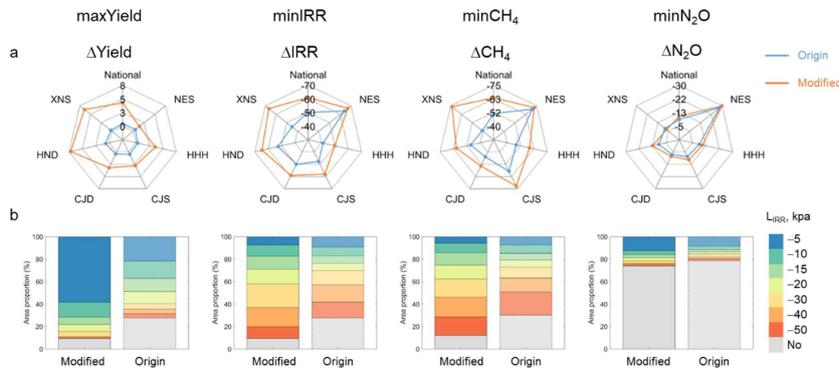
715 over 91%, 91%, 88% and 26% of national rice areas (Fig. 5b6b). Spatially, larger  
716 yield increase potential occurred in south (HND: 7.7%) and southwest regions (XNS:  
717 6.8%) (Fig. S9AS12A). The reduction potential of IRR and CH<sub>4</sub> showed relatively  
718 slight spatial variabilities. In contrast, reduction potential of N<sub>2</sub>O primarily  
719 concentrated in northern regions (NES: -30%) due to increased N<sub>2</sub>O in southern  
720 regions (Fig. 5a and S9AS12A). N<sub>2</sub>O increase in southern regions is associated with  
721 higher nitrogen application rates, providing substrate for nitrification and  
722 denitrification processes to facilitate N<sub>2</sub>O emissions (Jiang et al., 2019). The results  
723 conform to previous studies in that irrigation and nitrogen should be co-regulated for  
724 these areas to avoid unintended N<sub>2</sub>O emissions from water management (Jiang et al.,  
725 2019; Kritee et al., 2018).

726  
727 The largest regulation potentials of  $\Delta$ Yield,  $\Delta$ IRR,  $\Delta$ CH<sub>4</sub>, and  $\Delta$ N<sub>2</sub>O are not likely to  
728 be achieved at the same time, as evidenced by different optimized irrigation strategies  
729 between single-objective targets (Fig. 5-6 and S10S13). For example, the lower  
730 irrigation threshold should be higher than -20kpa for most areas (84%) under  
731 *maxYield*, while lower than -20kpa over half areas under *minIRR* and *minCH<sub>4</sub>*. This  
732 suggests tradeoffs between yield increase and IRR/CH<sub>4</sub> mitigation (Bo et al., 2021).  
733 To compare, using the origin model could overlook nearly 20% feasible areas for  
734 applying optimized irrigation schemes (Fig. 56). As a consequence, regulation  
735 potentials of  $\Delta$ Yield,  $\Delta$ IRR,  $\Delta$ CH<sub>4</sub> and  $\Delta$ N<sub>2</sub>O could be underestimated by 4%, 11%,  
736 14%, and 2%, especially for the southwest regions (XNS) (Fig. 5a6a). Moreover,  
737 optimal NCF strategies also differed from that identified by the improved model,  
738 particular under *maxYield* targets (Fig. 5b6b). These results showed important  
739 implications of the improved framework for prompting sustainable water  
740 management.  
741 -



742 =  
743 **Figure 4** Spatial pattern of relative changes in target variables under different  
744 irrigation schemes and differences. The four columns correspond to the four target  
745 variables  $\Delta$ Yield,  $\Delta$ IRR,  $\Delta$ CH<sub>4</sub>, and  $\Delta$ N<sub>2</sub>O, respectively. (a) relative changes of target  
746 variables under a lower irrigation potential of -15 kpa, (a) relative changes of target  
747 variables under a lower irrigation potential of -30 kpa, (c) differences between (b) and  
748 (a), (d) results for different rice growing regions. NES, HHH, CJS, CJD, HND, and  
749 XNS indicate six rice growing areas of China, namely, Northeast Single rice,  
750 HuangHuaiHai single rice, Yangtze River single rice, Yangtze River double Rice, South  
751 China Double rice, and Southwest China Single rice, respectively.

752  
753



754  
755 **Figure 65 Comparison of the origin and modified model from (a) regulation**  
756 **potentials and (b) optimized irrigation schemes under single-objective targets.**  
757 The four columns show results under four single objective targets: maximizing rice  
758 yield (*maxYield*), minimizing irrigation water use (*minIRR*), minimizing CH<sub>4</sub>  
759 emissions (*minCH<sub>4</sub>*), and minimizing N<sub>2</sub>O emissions (*maxN<sub>2</sub>O*). **(a)** Area-weighted  
760  $\Delta$ Yield,  $\Delta$ IRR,  $\Delta$ CH<sub>4</sub>, and  $\Delta$ N<sub>2</sub>O for China and six rice growing regions. Blue and  
761 orange indicate results from the origin and modified model, respectively. **(b)**  
762 Proportions of rice areas with corresponding optimized lower irrigation thresholds  
763 ( $L_{IRR}$ ) to total irrigated rice areas under the four single objective targets. NES, HHH,  
764 CJS, CJD, HND, and XNS indicate six rice growing areas of China, namely,  
765 Northeast Single rice, HuangHuaiHai single rice, Yangtze River single rice, Yangtze  
766 River double Rice, South China Double rice, and Southwest China Single rice,  
767 respectively.

### 768 3.4 Tradeoffs between food, water, and greenhouse gas emissions

771 The NSGA-II algorithm was conducted to investigate synergies or tradeoffs of the food-  
772 water-climate nexus (Fig. 6-7 and Section 2.6). There were evident tradeoffs between  
773 reducing CH<sub>4</sub> (or IRR) and N<sub>2</sub>O (Fig. 6a7a). In contrast, synergies were noted between  
774 reducing IRR and CH<sub>4</sub>, as well as between inhibiting N<sub>2</sub>O emissions and increasing rice  
775 yield. The relationships between yield increase and CH<sub>4</sub> (or IRR) reductions were more  
776 complicated due to the impacts of varying irrigation timing and no-flooded days (Yan  
777 et al., 2024). Adopting non-dominated solutions from multi-objective optimization  
778 could realize over 90% of the largest reduction potentials of IRR and CH<sub>4</sub>, while at the  
779 cost of 4% less yield increase (4.6% versus 0.5%) and 25% higher nitrous dioxide  
780 emissions (-11% versus 14%). The N<sub>2</sub>O increase is because this study used integrated  
781 warming potentials of CH<sub>4</sub> and N<sub>2</sub>O emissions (GWP) to indicate greenhouse gas  
782 emissions so that CH<sub>4</sub> outweighed N<sub>2</sub>O due to large emission quantities (Section 2.6).

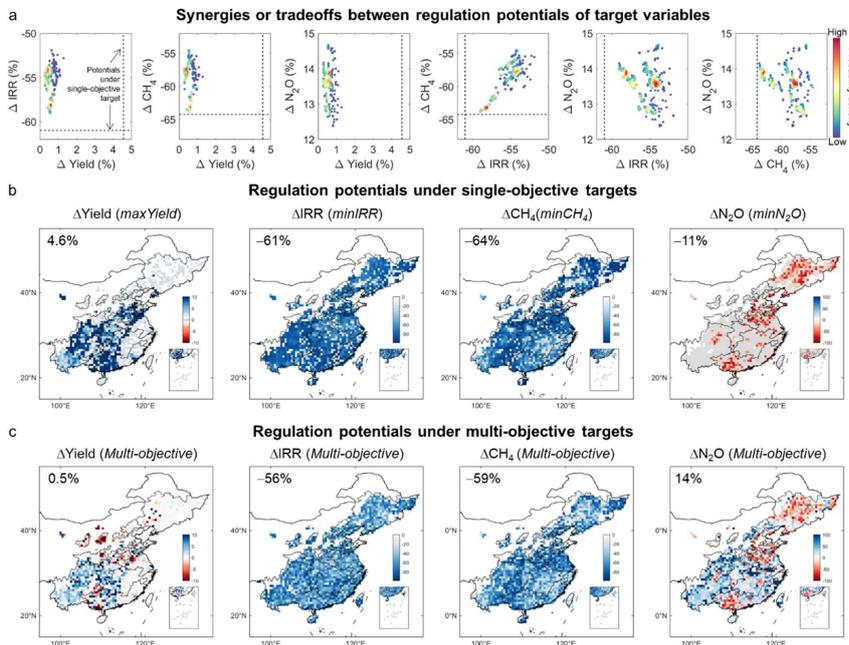
783  
784 **Spatially, over 90% of the reduction potentials for IRR and CH<sub>4</sub> could be achieved**  
785 **across 53% and 60% of the national rice areas, primarily in southern regions (Fig. 7 and**  
786 **S14). In these areas, N<sub>2</sub>O increase was inevitable, but yield increase could be expected.**

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787 By contrast, stronger tradeoffs occurred in the northern regions, where the reduction  
 788 potentials of IRR and CH<sub>4</sub> were limited even with decreased yield and increased N<sub>2</sub>O  
 789 emissions. Therefore, NCF adoption should be prioritized in southern regions (e.g.  
 790 XND, CJD, CJS) to achieve Since the multi-objective optimization was conducted  
 791 targeting a national optimum balance among rice production, water use, and greenhouse  
 792 gas emissions mitigation of food-water-GHGs, NCF practices were adopted in the south  
 793 regions to realize more considerable IRR and CH<sub>4</sub> reductions contributing to larger  
 794 national co-benefits. Noted that other objective functions could also be designed for  
 795 multi-objective optimization, such as applying other indicators (e.g., water productivity,  
 796 yield-scaled GWP), setting distinguished weights for each indicator or grid cell.  
 797



798 **Figure 6-7** Regulation potentials of  $\Delta$ Yield,  $\Delta$ IRR,  $\Delta$ CH<sub>4</sub>, and  $\Delta$ N<sub>2</sub>O under single-  
 799 **objective and multi-objective targets.** (a) Synergies or tradeoffs between target  
 800 variables with different solutions of multi-objective optimization. Dots color indicates  
 801 probability density distributions of variable changes from all non-dominated solutions  
 802 (N = 10000) of the NSGA II optimization. The vertical and horizontal dashed lines  
 803 show national regulation potentials of the target variable under single-objective  
 804 targets, with corresponding spatial distributions presented in panel (b). Note that the  
 805 results of  $\Delta$ N<sub>2</sub>O potentials (-11%) were not shown in the third, fifth, and sixth  
 806 subplots for a clearer view. (b)  $\Delta$ Yield,  $\Delta$ IRR,  $\Delta$ CH<sub>4</sub>, and  $\Delta$ N<sub>2</sub>O under single-objective  
 807 targets of maximizing rice yield (*maxYield*), minimizing irrigation water use  
 808 (*minIRR*), minimizing CH<sub>4</sub> emissions (*minCH<sub>4</sub>*), and minimizing N<sub>2</sub>O emissions  
 809 (*maxN<sub>2</sub>O*). These results indicate the maximum benefits of each target variable from  
 810

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811 adopting non-continuous irrigation, which could not be necessarily realized  
812 simultaneously. (c)  $\Delta$ Yield,  $\Delta$ IRR,  $\Delta$ CH<sub>4</sub>, and  $\Delta$ N<sub>2</sub>O under multi-objective  
813 optimization. These figures show mean benefits from all non-dominated solutions of  
814 the NSGA II optimization (N = 10000).

815

### 816 3.5 Uncertainties and future direction

817

818 This framework is subject to several uncertainties, mainly sourced from observational  
819 gaps and management-related input data. First, the absence of field observations for  
820 baseline CH<sub>4</sub> and N<sub>2</sub>O emissions across regional scales forced us to use estimates from  
821 inventory or data-driven approaches as a proxy for deriving gridded model parameters  
822 of this study (Cui et al., 2021; Crippa et al., 2024). Despite uncertainties in predicting  
823 absolute values, these parameters could reasonably reproduce the spatial patterns and  
824 could be further refined given increased field observations. Second, the limited  
825 experimental observations of CH<sub>4</sub> ( $n = 37$ ) and N<sub>2</sub>O ( $n = 14$ ) under various irrigation  
826 schemes have contributed to uncertainties in developing and applying parameter  
827 transfer functions (PTFs). The values of PTFs predictors (bulk density and field water  
828 capacity) in the observation dataset (1.34~1.48 g cm<sup>-3</sup> and 0.25~0.30 cm<sup>3</sup> cm<sup>-3</sup>) did not  
829 encompass the full range across national rice areas (1.24~1.48 g cm<sup>-3</sup> and 0.22~0.32  
830 cm<sup>3</sup> cm<sup>-3</sup>), indicating potential extrapolation in parameters regionalization (Fig. S1).  
831 Despite these uncertainties, the PTFs significantly improved over previous approaches  
832 (constant parameters or spatial proximity approach). Lastly, current irrigation practices  
833 across large scales remain largely unknown, so that irrigation thresholds were set  
834 following previous recommendations. However, actual farmer practices are influenced  
835 by various factors and may not align with these recommendations. This discrepancy  
836 could lead to an overestimation or underestimation of target variables and further  
837 introduce uncertainties to the assessment of regulation potentials.

838

839 These uncertainties provide insights to enlighten future research efforts, including  
840 conducting extensive observations and experiments and developing high-resolution  
841 input data. On the one hand, intensive GHGs monitoring networks are essential to  
842 reduce uncertainties associated with parametrization (Arenas-Calle et al., 2024). To  
843 better constrain the PTFs and reduce extrapolation uncertainty, field experiments  
844 combined with incubation experiments covering across a broader range of climate  
845 conditions (e.g., colder and more humid areas) and soil properties (e.g., areas with  
846 higher SOC or lower bulk density), including bulk density and field water capacity,  
847 should be conducted (Fig. S1). In addition, extensive field experiments with  
848 simultaneous measurements of yield, IRR, CH<sub>4</sub>, and N<sub>2</sub>O emissions across diverse  
849 environments are required to validate the framework further. On the other hand,  
850 developing a high-resolution dataset of current irrigation schemes is crucial for more  
851 accurate model parameter calibration and realistic assessment of regulation potentials.  
852 This could be achieved by integrating remote sensing technologies with extensive field  
853 investigations (Novick et al., 2022).

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855 **4 Conclusion**

856

857 This study introduced an advancing framework for process-based modelling of the  
 858 complex food-water-climate nexus in rice fields under various water management  
 859 schemes. By integrating the Soil Water Heat Carbon Nitrogen Simulator (WHCNS)  
 860 with key physiological effects, a novel model upscaling method, and the NSGA-II  
 861 multi-objective optimization algorithm at a parallel computing platform, the framework  
 862 provides a comprehensive approach to optimize irrigation strategies. Applying this  
 863 framework to China’s rice cropping system, we assessed the largest regulation  
 864 potentials of  $\Delta$ Yield,  $\Delta$ IRR,  $\Delta$ CH<sub>4</sub>, and  $\Delta$ N<sub>2</sub>O as 4.6%, -61.0%, -64.2%, and -10.9%  
 865 from 91%, 91%, 88%, and 26% of national rice areas. However, these regulation  
 866 potentials could not be simultaneously realized due to complicated tradeoffs among  
 867 food-water-GHGs. Based on NSGA II multi-objective optimization targeting food-  
 868 water-GHGs co-benefits, over 90% of the reduction potentials in water use and methane  
 869 emissions could be realized, while at the cost of 4% less yield increase and 25% higher  
 870 nitrous dioxide emissions. The proposed framework is a valuable tool for irrigation  
 871 optimization in rice cultivation and also offers a transferable paradigm for incorporating  
 872 other management effects into process-based models, thus supporting comprehensive  
 873 assessments of sustainable management measures.

874

875 **Appendix: abbreviation table**

876

Type	Abbreviation	Description
Target variables	<i>Yield</i>	<del>R</del> ice yield (kg ha <sup>-1</sup> )
	<i>IRR</i>	<del>irrigation-Irrigation</del> water use (mm)
	<i>CH<sub>4</sub></i>	<del>methane-Methane</del> emissions (kg ha <sup>-1</sup> )
	<i>N<sub>2</sub>O</i>	<del>nitrous-Nitrous</del> oxide emissions (kg ha <sup>-1</sup> )
	<i>GWP</i>	<del>integrated-Integrated</del> global warming potential of CH <sub>4</sub> and N <sub>2</sub> O at 100-year scale, calculated as 27.2×CH <sub>4</sub> +273×N <sub>2</sub> O (kg ha <sup>-1</sup> )
	<i>LAI</i>	<del>leaf-Leaf</del> area index (m <sup>2</sup> m <sup>-2</sup> )
	<i>Pn</i>	<del>net-Net</del> photosynthetic rate (kg ha <sup>-1</sup> )
Effect sizes	<i>HI</i>	<del>harvest-Harvest</del> index (-)
	<i>R<sup>Yield</sup>, R<sup>IRR</sup>, R<sup>CH<sub>4</sub></sup>, R<sup>N<sub>2</sub>O</sup>, R<sup>LAI</sup>, R<sup>Pn</sup>, R<sup>HI</sup></i>	Effect size of non-continuous flooding irrigation (NCF) on target variables, calculated as the ratio of observations under NCF to that under continuous flooding (CF) (-)
Relative changes	<i>ΔYield, ΔIRR, ΔCH<sub>4</sub>, ΔN<sub>2</sub>O</i>	Relative changes of target variables under NCF compared to CF, calculated as (R-1)×100 (%)
Model parameters	<i>Cumtemp</i>	accumulated temperature for crop maturity (°C)
	<i>AMIN</i>	<del>minimum-Minimum</del> assimilation rates (kg hm <sup>-2</sup> h <sup>-1</sup> )
	<i>p<sup>LAI</sup>, p<sup>Pn</sup>, p<sup>HI</sup></i>	<del>genetic-Genetic</del> parameters accounting for cultivar sensitivities to NCF effects on leaf area

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		index, net photosynthetic rate, and harvest index
	<i>MPmax</i>	<del>maximum</del> - <b>Maximum</b> CH <sub>4</sub> production rate per soil weight at 30 °C (g C g <sup>-1</sup> d <sup>-1</sup> )
	<i>f<sub>N<sub>2</sub>O,d</sub></i>	<del>maximum</del> - <b>Maximum</b> portion of denitrification to N <sub>2</sub> O production (-)
Environmental variables	<i>T</i>	<del>mean</del> - <b>Mean</b> daily air temperature during rice growing season (°C)
	<i>P</i>	<del>total</del> - <b>Total</b> precipitation during rice growing season (mm)
	<i>PETc</i>	<del>total</del> - <b>Total</b> crop evapotranspiration during rice growing season (mm)
	<i>CWA</i>	<del>climatological</del> - <b>Climatological</b> water availability, calculated as the difference between <i>P</i> and <i>PETc</i> ( <i>P</i> - <i>PETc</i> , mm)
Soil variables	<i>BD</i>	<del>bulk</del> - <b>Bulk</b> density (g cm <sup>-3</sup> )
	<i>Sand</i>	<del>sand</del> - <b>Sand</b> content (%)
	<i>Clay</i>	<b>Clay content (%)</b>
	<i>SOC</i>	<del>soil</del> - <b>Soil</b> organic carbon (%)
	<i>SAT</i>	<del>saturated</del> - <b>Saturated</b> water content (cm <sup>3</sup> cm <sup>-3</sup> )
	<i>FWC</i>	<b>F</b> ield water capacity (cm <sup>3</sup> cm <sup>-3</sup> )
Management variables	<i>L<sub>AWD</sub></i>	<del>lower</del> - <b>Lower</b> irrigation threshold, indicated by SWP (kpa)
	<i>U<sub>AWD</sub></i>	<del>upper</del> - <b>Upper</b> irrigation threshold (cm)
	<i>SWP</i>	<del>soil</del> - <b>Soil</b> water potential (kpa)
	<i>UFR</i>	<del>ratio</del> - <b>Ratio</b> of unflooded days to total growing days (%)
Optimization objectives	<i>maxYield</i>	<del>maximizing</del> - <b>Maximizing</b> rice yield
	<i>minIRR</i>	<del>minimizing</del> - <b>Minimizing</b> irrigation water use
	<i>minCH<sub>4</sub></i>	<del>minimizing</del> - <b>Minimizing</b> CH <sub>4</sub> emission
	<i>minN<sub>2</sub>O</i>	<del>minimizing</del> - <b>Minimizing</b> N <sub>2</sub> O emissions

877

#### 878 **Code and data availability**

879 The ~~executable~~-**origin code** of WHCNS model and required model input files are

880 available at <https://figshare.com/s/139f3ad8a70faa99724d>. Spatial dataset of

881 harvested area of irrigated rice is available from

882 <https://doi.org/10.7910/DVN/KAGRFI>. **Origin c**limate data is available from—

883 <https://cds.climate.copernicus.eu/datasets/reanalysis-era5-single->

884 [levels?tab=downloadhttps://cds.climate.copernicus.eu/edsapp#!search?type=dataset.](https://cds.climate.copernicus.eu/edsapp#!search?type=dataset)

885 **Origin S**oil data ~~are is~~ available from [https://doi.org/10.1002/2013MS000293-](https://doi.org/10.1002/2013MS000293)

886 <http://globalchange.bnu.edu.cn/research/data>. **Processed climate and soil data for**

887 **model running are included in the figshare repository (see Readme for detailed**

888 **explanations of each file)**. Crop calendar data are available from—

889 <https://zenodo.org/record/5062513>. All other data that support the findings of this

890 study are available in the main text or the Supplementary Information.

891

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895

### 896 **Author contributions**

897 F.Z. designed the study. Y.B. and H.L. performed all computational analyses. Y.B.,  
898 H.L. and F.Z. drafted the paper. Y.B., H.L., T. L. and F.Z. reviewed and commented on  
899 the manuscript.

900

### 901 **Conflict of interest statement**

902 The authors declare no conflicts of interest.

903

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