Supplementary Materials

Revealing Climate-Induced Patterns in Crop Yields and the Water-Energy-Food-Carbon Nexus: Insights from the Pearl River Basin

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This Supplementary Materials file includes:

Section 1 Sobol Sensitivity analysis method

Section 2 Rules-based irrigation strategies

Section 3 Mann-Kendall test

Section 4: Supplementary Tables S1–S9

Section 5: Supplementary Figures S1–S10

References

Section 1 Sobol sensitivity analysis method

This method can be represented by the following equation:

$$Y = f(X) = f(X_1, X_2, \cdots, X_n)$$

Specifically, the model output variable Y is crop yield, measured in $t \cdot hm^{-2}$, and $X = (X_1, X_2, \cdots, X_n)$ represents the model parameter values. The total variance $D(y)$ of the function $f(X)$ can be decomposed into several components as follows:

$$D(y) = \sum_i D_i + \sum_{i<j} D_{ij} + \cdots + D_{12\cdots n}$$

Here, D_i is the variance contribution of the *i*-th parameter X_i, D_{ij} is the variance contribution of the interaction between parameters X_i and X_j, and $D_{12\cdots n}$ is the variance contribution from the interaction of all parameters. The sensitivity indices are calculated as the ratio of these variance contributions to the total variance $D(y)$, providing insights into the individual and interaction effects of the parameters.

First-order sensitivity index:

$$S_i = \frac{D_i}{D(y)}$$

Total sensitivity index:

$$S_{Ti} = 1 - \frac{D_{\sim i}}{D(y)}$$

Where, $D_{\sim i}$ represents the variance of the output excluding the *i*-th parameter. In this study, we set the sample size for each crop to 1024, meaning that the sensitivity analysis for each crop requires running the model $1024\times\left(2\times19+2\right)$ times.

Section 2 Rules-based irrigation strategies

To ensure the irrigation strategy aligns more closely with real-world practices, we propose a rule-based irrigation strategy tailored for the Pearl River Basin. The irrigation strategy developed in this study determines the necessity for irrigation based on the crop growth stages, soil moisture conditions, and irrigation frequency. This approach helps to avoid unnecessary irrigation following periods of rainfall and aims to closely match the actual irrigation practices in the Pearl River Basin.

For rice:

$$Irr_{rice} = \begin{cases} irr, & if\ \left(0 < t < t_1\ and\ soil_{hydro} < thresholds_{Emergence}\ and\ t_{cal} < t_{irr}\right) \\ irr, & if\ \left(t_1 < t < t_2\text{-}6\ and\ soil_{hydro} < thresholds_{Early\ Vegetative}\ and\ t_{cal} < t_{irr}\right) \\ 0, & if\ \left(t_2\text{-}6 < t < t_2\ and\ soil_{hydro} < thresholds_{Mid\ Vegetative}\ and\ t_{cal} < t_{irr}\right) \\ irr, & if\ \left(t_2 < t < t_3\ and\ soil_{hydro} < thresholds_{Late\ Vegetative}\ and\ t_{cal} < t_{irr}\right) \\ irr, & if\ \left(t_3 < t < t_4\ and\ soil_{hydro} < thresholds_{Reproductive}\ and\ t_{cal} < t_{irr}\right) \\ irr, & if\ \left(t_4 < t < t_5\text{-}8\ and\ soil_{hydro} < thresholds_{Grain\ Filling}\ and\ t_{cal} < t_{irr}\right) \\ 0, & if\ \left(t_5\text{-}8 < t < t_5\ and\ soil_{hydro} < thresholds_{Maturity}\ and\ t_{cal} < t_{irr}\right) \end{cases}$$

Where irr represents the irrigation amount per event, in mm; t is the crop growth duration, in days; t_1 to t_5 represent different growth stages and can be referenced from Supplementary Table S3; It is important to note that $t_2{-}6$ to t_2 correspond to the late tillering stage, where irrigation is usually stopped; $t_5{-}8$ to t_5 represent the pre-harvest stage, where irrigation is ceased to ensure crop ripening; $soil_{hydro}$ represents the soil hydrological condition on day t; *thresholds* are the conditions that trigger irrigation; t_{irr} is the minimum number of

days between subsequent irrigation events, for rice, it is 3 days.

For maize：

$$Irr_{maize}=\begin{cases} irr, & if\ \left(0<t<t_1\ and\ soil_{hydro}<thresholds_{Emergence}\ and\ t_{cal}<t_{irr}\right) \\ irr, & if\ \left(t_1<t<t_2\ and\ soil_{hydro}<thresholds_{Early-Mid\ Vegetative}\ and\ t_{cal}<t_{irr}\right) \\ irr, & if\ \left(t_2<t<t_3\ and\ soil_{hydro}<thresholds_{Late\ Vegetative}\ and\ t_{cal}<t_{irr}\right) \\ irr, & if\ \left(t_3<t<t_4\ and\ soil_{hydro}<thresholds_{Reproductive}\ and\ t_{cal}<t_{irr}\right) \\ irr, & if\ \left(t_4<t<t_5\text{-}15\ and\ soil_{hydro}<thresholds_{Grain\ Filling}\ and\ t_{cal}<t_{irr}\right) \\ 0, & if\ \left(t_5\text{-}15<t<t_5\ and\ soil_{hydro}<thresholds_{Maturity}\ and\ t_{cal}<t_{irr}\right) \end{cases}$$

We set t_{irr} to 5 days because the irrigation frequency for maize is lower than that for rice.

$$tcal=\begin{cases} 0, & if\ irr_{crop}=irr \\ tcal+1, & if\ irr_{crop}=0 \end{cases}$$

Section 3 Mann-Kendall test

The detailed calculations are as follows:

$$\operatorname{sgn}(\theta)=\begin{cases}1, & \theta>0\\ 0, & \theta=0\\ -1, & \theta<0\end{cases}$$

$$S=\sum_{i=1}^{n-1}\sum_{k=i+1}^{n}\operatorname{sgn}\left(x_k-x_i\right)$$

$$Var(S)=\frac{1}{18}\left[n(n-1)(2n+5)-\sum_t t(t-1)(2t+5)\right]$$

$$Z_c=\begin{cases}\dfrac{S-1}{\sqrt{Var(S)}}, & if\ S>0\\ 0, & if\ S=0\\ \dfrac{S+1}{\sqrt{Var(S)}}, & if\ S<0\end{cases}$$

Where, x_k and x_i are the values in years k and i. n is the length of the time series. t is the number of tied groups. The trend Z_C indicates the direction of the trend over time, with positive values indicating an increasing trend and negative values indicating a decreasing trend. A trend is considered significant if $|Z_C|\geq Z_1-\alpha/2$, where $|Z_C|\geq Z_1-\alpha/2$ is the critical value from the standard normal distribution. In this study, a significance level of 99% is selected, thus $|Z_C|\geq Z_1-\alpha/2=2.56$。

Section 4 Supplementary Tables

Supplementary Table S1 Performance Metrics for Different Meteorological Variables under MME

name	pearson_r	crmse	sdev
hurs	0.96	0.29	1.03
ps	0.98	0.19	1.00
rds	0.89	0.47	0.97
sfcwind	0.74	0.72	1.01
tasmax	0.94	0.34	1.02
tasmin	0.95	0.33	1.00
pr	0.86	0.51	1.11

Note: the evaluation metrics—Pearson correlation coefficient (r), centered root mean square error (cRMSE), and standard deviation ($sdev$)—for various meteorological variables simulated by the MME in the Pearl River Basin. The variables assessed include relative humidity (hurs), surface pressure (ps), radiation (rds), surface wind speed (sfcwind), maximum temperature (tasmax), minimum temperature (tasmin), and precipitation (pr).

Supplementary Table S2 Average hydrological data of the watershed soil

Depth (cm)	WP (%)	FC (%)	Sat (%)	Ksat (cm/d)
4.5	0.20	0.34	0.51	21.67
9.1	0.20	0.34	0.50	21.34
16.6	0.20	0.34	0.50	20.00
28.9	0.20	0.34	0.49	16.77
49.3	0.22	0.35	0.49	12.99
82.9	0.22	0.35	0.47	10.15
138.3	0.22	0.35	0.47	10.15

Note: Depth is Soil depth from the surface; WP is Wilting Point - the minimal soil moisture at which a plant wilts and cannot recover; FC is Field Capacity - the amount of soil moisture or water content held in the soil after excess water has drained away; Sat is Saturation Point - the maximum amount of water content that the soil can hold; Ksat is Saturated Hydraulic Conductivity - the ease with which pores of a saturated soil transmit water.

Supplementary Table S3 Irrigation thresholds for rice and maize

Crop	Flooded irrigation	Emergence	Early Vegetative	Mid Vegetative	Late Vegetative	Reproductive	Grain Filling	Maturity
Rice	yes	15mm	15mm	dry	25mm	15mm	15mm	dry
Maize	no	80%	80%	80%	85%	85%	75%	dry

Notes: Flooded Irrigation Indicates whether the crop requires flooded irrigation. If it is flood irrigation, the threshold for triggering irrigation is the depth of the surface water layer; if not, it is the soil moisture content; **Emergence** Represents the irrigation threshold during the emergence stage. Both rice and maize means seeding; **Early Vegetative** Indicates the irrigation requirement during the early vegetative stage. For rice, it means tillering, and for maize, it means V3 stage; **Mid Vegetative** Specifies the irrigation requirement during the mid vegetative stage. Both rice and maize means stem elongation; **Late Vegetative** Indicates the irrigation threshold during the late vegetative stage. For rice, it means panicle initiation, and for maize, it means tasseling; **Reproductive** Represents the irrigation requirement during the reproductive stage. For rice, it means heading and flowering, and maize means silking; **Grain Filling** Specifies the irrigation requirement during the grain filling stage. Both rice and maize mean milking; **Maturity** Indicates the irrigation requirement during the maturity stage. Both crops require dry conditions.

Supplementary Table S4 Price of inputs in crop production

year	Plastic film (yuan/kg)	Pestiside (yuan/kg)	Diesel fuel (yuan/kg)	Electricity (yuan/kwh)	labor cost (yuan/day)	Machinery cost (yuan/day)
2000	8.5	15.76833	2.983333	0.390767	41.78937	32.9916
2001	9.23	15.69611	3.238333	0.390767	42.62515	33.65144
2002	8.988333	19.67433	3.061667	0.390767	42.62515	33.65144
2003	8.534167	19.28967	3.64	0.390767	41.3464	32.64189
2004	8.534167	17.29	3.8175	0.375933	43.95122	34.69833
2005	11.64917	20.82067	4.699167	0.375933	48.08264	37.95998
2006	12.84083	21.41367	5.211667	0.348333	50.87143	40.16165
2007	13.49167	22.5865	5.68625	0.348333	52.60106	41.52715
2008	14.71458	28.09583	6.945833	0.348333	56.86174	44.89085
2009	13.48542	24.336	6.433333	0.348333	58.28329	46.01312
2010	13.78625	24.01767	7.405	0.348333	62.47968	49.32607
2011	14.24042	24.75417	8.44875	0.348333	67.54054	53.32148
2012	14.205	26.87417	8.8	0.348333	71.52543	56.46744
2013	14.759	27.33103	8.844	0.370975	76.17458	60.13783
2014	15.06893	27.68633	8.684808	0.385814	79.22157	62.54334
2015	15.18949	27.82476	7.581837	0.394302	80.96444	63.91929
2016	15.1743	27.82476	7.324055	0.400216	82.17891	64.87808
2017	15.28052	28.10301	8.05646	0.40622	83.41159	65.85126
2018	15.47916	29.53626	9.071574	0.417594	85.74711	67.69509
2019	15.61848	30.48142	8.581709	0.427198	87.7193	69.25208
2020	15.3842	31.15202	8.942141	0.462656	95	75

Supplementary Table S5 Energy equivalents of inputs in crop production

Items	Unit	Energy equivalent (MJ unit−1)	Reference
Human labor	person·h	1.96	(Du et al., 2023)
Machinery	set·h	62.7	(Du et al., 2023)
Nitrogen	kg	66.14	(Yuan & Peng, 2017)
Phosphorus	kg	12.44	(Yuan & Peng, 2017)
Potassium	kg	11.15	(Yuan & Peng, 2017)
Compound fertilizer	kg	12.83	(Yuan & Peng, 2017)
Pestiside	kg	100.34	(He et al., 2022)
Electricity	kWh	3.6	(Yuan & Peng, 2017)
Diesel fuel	kg	43.51	(Feng et al., 2023)
Plastic film	kg	154.72	(He et al., 2022)

Water	m^3	1.02	(Du et al., 2023)
Rice seed	kg	15.97	(Feng et al., 2023)
Maize seed	kg	16.49	(Feng et al., 2023)

Supplementary Table S6 Carbon emission factors of inputs in crop production

Items	Unit	Emission factor (kg CE unit-1)	Reference
Human labor	person/ha·h	0.03	(Kumar et al., 2021)
Machinery	set/ha·h	0.89	(Kumar et al., 2021)
Nitrogen	kg	7.76	(Gu et al., 2024)
Phosphorus	kg	2.33	(Gu et al., 2024)
Potassium	kg	0.66	(Gu et al., 2024)
Compound fertilizer	kg	1.44	(He et al., 2022)
Pestiside	kg	10.44	(Gu et al., 2024)
Electricity	kWh	0.439	(He et al., 2022)
Diesel fuel	kg	3.58	(He et al., 2022)
Plastic film	kg	5.18	(He et al., 2022)
Water	m^3	0.17	(Du et al., 2023)
Seed	kg	0.32	(Du et al., 2023)

Supplementary Table S7 Default values of parameters used in the calculation of CH_4 and N_2O emissions

GHG type	Parameter	Value	Source
CH_4	EF_c, $t \cdot CH_4 \cdot ha^{-1} \cdot day^{-1}$	1.320	(Calvo Buendia, E. et al., 2019)
	SF_W, %	0.710	(Calvo Buendia, E. et al., 2019)
	SF_P, %	1.000	(Calvo Buendia, E. et al., 2019)
	SF_o, %	1.210	(Calvo Buendia, E. et al., 2019)
	SF_s, %	1.000	(Calvo Buendia, E. et al., 2019)
	SF_r, %	1.000	(Calvo Buendia, E. et al., 2019)
N_2O	EF_{d-N_2O}, $kg \cdot N_2O-N \cdot kg^{-1}$	0.018~0.011	(Ministry of Environmental Protection of China, 2011)
	$Frac_{GASF}$, %	0.110	(Calvo Buendia, E. et al., 2019)
	EF_{GASF-N_2O}, $kg \cdot N_2O-N \cdot kg^{-1}$	0.010	(Calvo Buendia, E. et al., 2019)
	$Frac_L$, %	0.240	(Calvo Buendia, E. et al., 2019)
	EF_{L-N_2O}, $kg \cdot N_2O-N \cdot kg^{-1}$	0.011	(Calvo Buendia, E. et al., 2019)

Supplementary Table S8 Machine learning predictive features

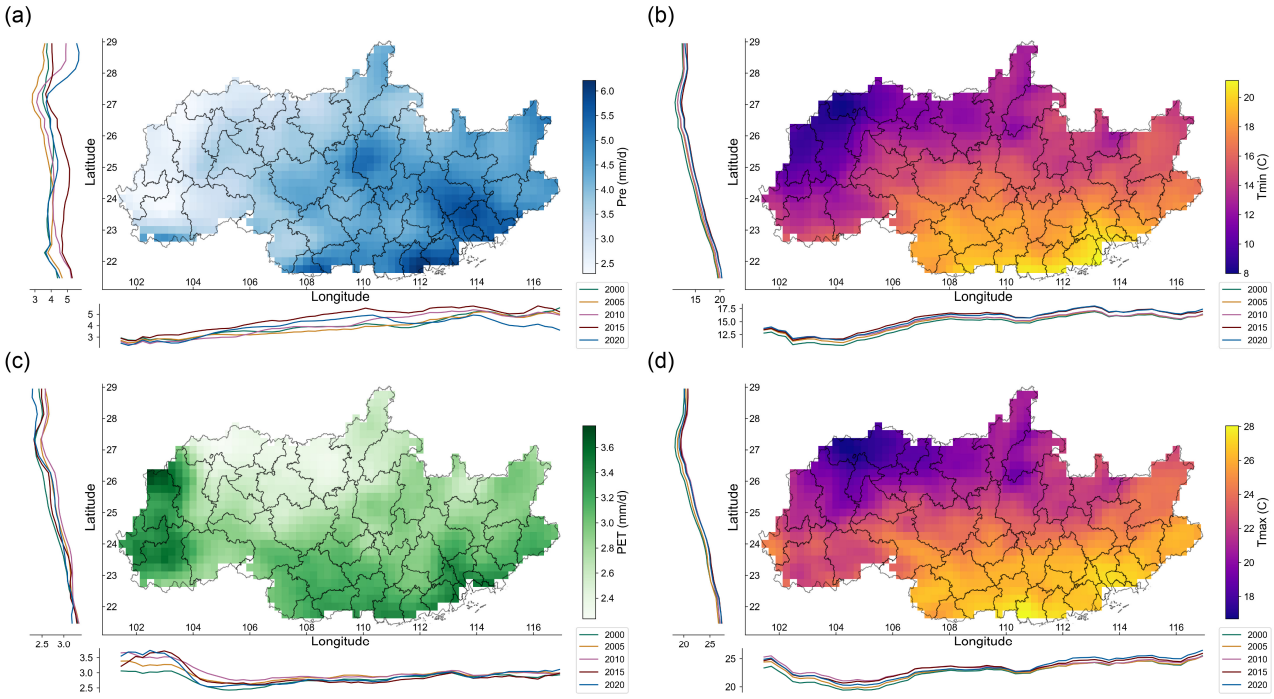
Variable	Name
sumpre	Total Precipitation
maxpre	Maximum Precipitation
tmax	Maximum Temperature
tmin	Minimum Temperature
sum30tm	Total Temperature Sum (≥ 30°C)
sum10tm	Total Temperature Sum (≥ 10°C)
sumtm	Total Temperature Sum
sumrn	Total Rainfall
sumet0	Total Reference Evapotranspiration
meanu2	Mean Wind Speed (at 2 meters)
maxu2	Maximum Wind Speed (at 2 meters)
meanrh	Mean Relative Humidity
lat	Latitude
lon	Longitude
dem	Digital Elevation Model (Elevation)

Supplementary Table S9 Comparative analysis of water, energy, and carbon footprints under different CO_2 concentration scenarios in the Pearl River Basin

Scenario	Year	CO_2 concentration in ISIMIP3b			Default CO_2 concentration in the AquaCrop model			RW (%)	RE (%)	RC (%)
		Water Footprint (m3/kg)	Energy Footprint (MJ/kg)	Carbon Footprint (kg/kg)	Water Footprint (m3/kg)	Energy Footprint (MJ/kg)	Carbon Footprint (kg/kg)			
ssp126	2021	0.69	8.72	1.98	0.69	8.73	1.98	-0.09	-0.09	-0.09
ssp126	2030	0.62	8.58	1.93	0.62	8.61	1.93	-0.29	-0.29	-0.29
ssp126	2040	0.66	8.49	1.90	0.65	8.47	1.90	0.27	0.27	0.27
ssp126	2050	0.58	8.37	1.87	0.58	8.25	1.84	1.46	1.42	1.42
ssp126	2060	0.67	8.41	1.88	0.65	8.17	1.82	3.18	2.87	2.87
ssp126	2070	0.61	8.36	1.87	0.58	7.99	1.79	5.56	4.45	4.42
ssp126	2080	0.65	8.51	1.89	0.61	7.99	1.77	6.78	6.15	6.14
ssp126	2090	0.67	8.60	1.91	0.60	7.83	1.74	9.85	9.00	8.98
ssp126	2100	0.61	8.58	1.92	0.52	7.58	1.69	14.14	11.72	11.68
ssp370	2021	0.73	8.67	1.97	0.73	8.70	1.98	-0.31	-0.31	-0.31
ssp370	2030	0.68	8.46	1.91	0.69	8.61	1.94	-1.76	-1.76	-1.76
ssp370	2040	0.72	8.31	1.86	0.75	8.58	1.92	-3.64	-3.28	-3.27
ssp370	2050	0.63	8.06	1.80	0.66	8.39	1.87	-4.89	-4.11	-4.09
ssp370	2060	0.55	7.87	1.74	0.59	8.36	1.84	-7.87	-6.20	-6.17
ssp370	2070	0.50	7.62	1.67	0.55	8.29	1.82	-10.05	-8.76	-8.73
ssp370	2080	0.63	7.68	1.66	0.71	8.56	1.85	-14.28	-11.48	-11.43
ssp370	2090	0.59	7.59	1.63	0.67	8.57	1.84	-14.65	-12.87	-12.84
ssp370	2100	0.47	7.34	1.57	0.55	8.39	1.79	-17.34	-14.29	-14.25
ssp585	2021	0.76	8.84	2.00	0.77	8.86	2.01	-0.25	-0.25	-0.25
ssp585	2030	0.69	8.63	1.93	0.70	8.79	1.97	-1.96	-1.82	-1.81
ssp585	2040	0.60	8.17	1.83	0.63	8.48	1.90	-4.30	-3.86	-3.85
ssp585	2050	0.49	7.97	1.76	0.52	8.42	1.86	-7.04	-5.67	-5.65
ssp585	2060	0.52	7.65	1.68	0.58	8.40	1.85	-11.28	-9.85	-9.83
ssp585	2070	0.58	7.71	1.66	0.68	8.82	1.90	-16.56	-14.36	-14.32
ssp585	2080	0.54	7.42	1.59	0.65	8.77	1.88	-22.04	-18.31	-18.25
ssp585	2090	0.51	7.29	1.55	0.63	8.75	1.86	-23.67	-19.97	-19.91
ssp585	2100	0.43	7.16	1.52	0.55	8.61	1.83	-28.24	-20.28	-20.17

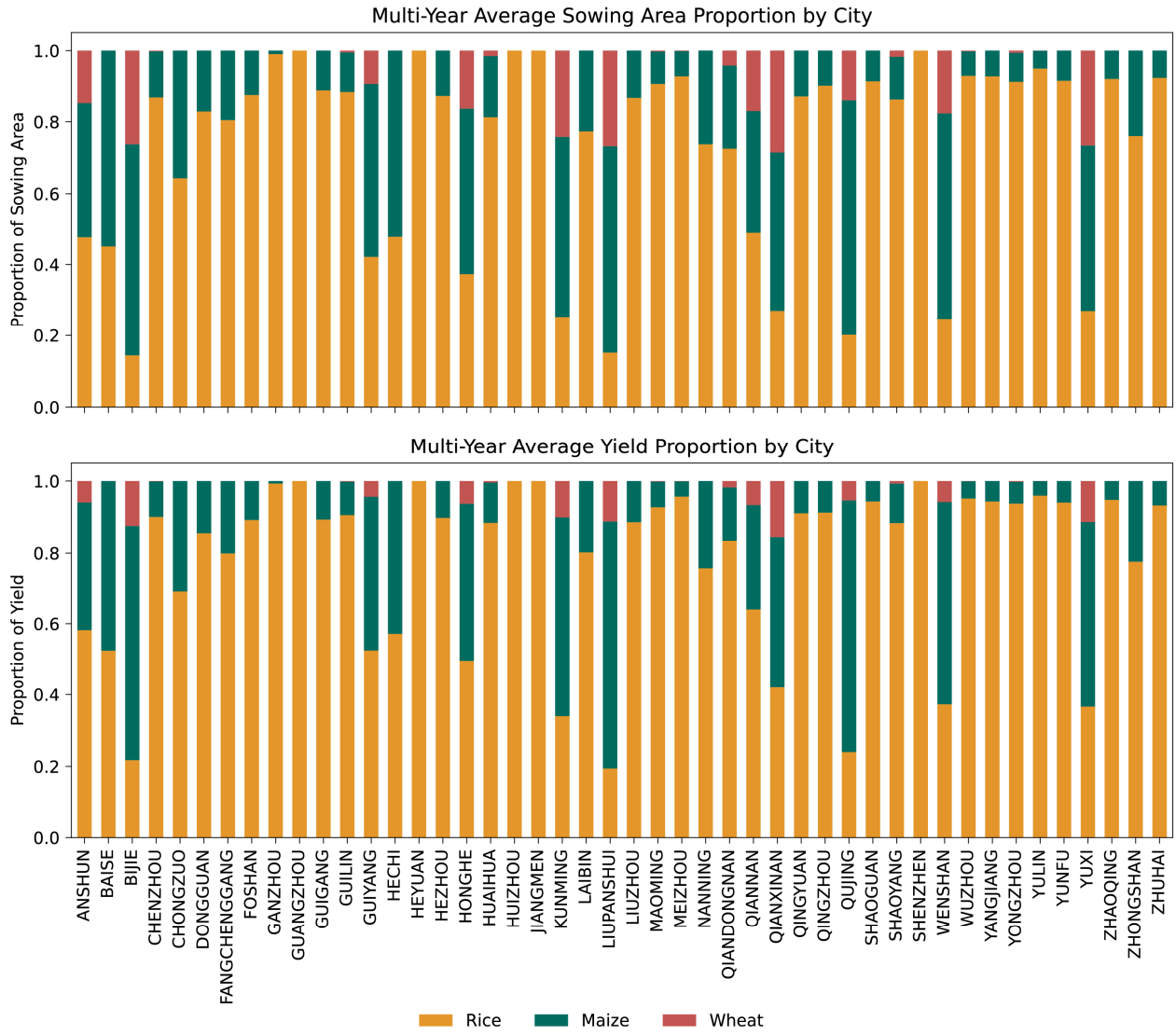
Note: This supplementary table presents a comparative analysis of the water, energy, and carbon footprints for agricultural production in the Pearl River Basin under different CO_2 concentration scenarios derived from ISIMIP3b and the default CO_2 concentrations in the AquaCrop model. The table includes data across various SSP scenarios and years, showing how changes in CO_2 concentrations impact the sustainability metrics of water, energy, and carbon footprints. The relative changes (RW, RE, RC) indicate the percentage differences in water, energy, and carbon footprints when comparing the ISIMIP3b CO_2 concentrations to the default concentrations in AquaCrop.

Section 5 Supplementary Figures

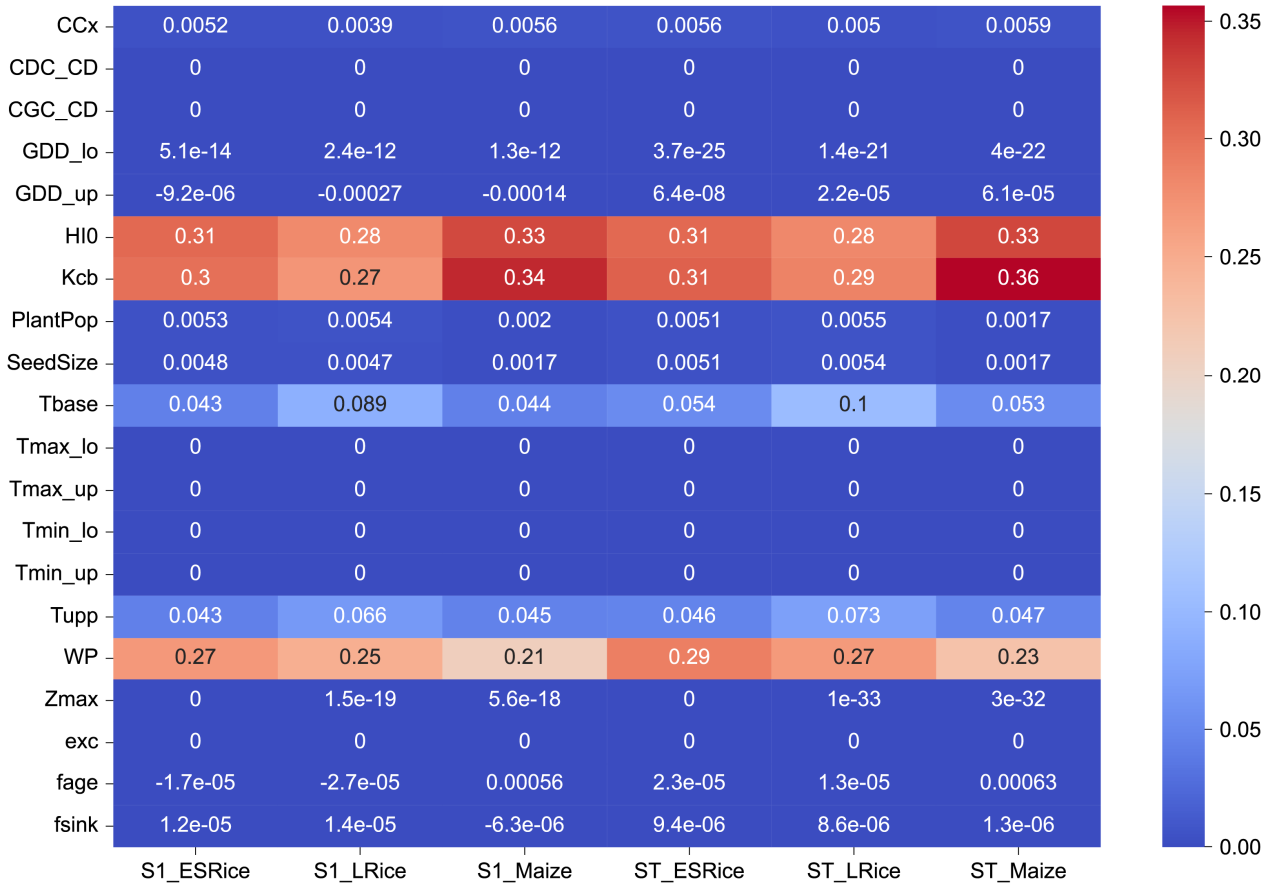


Supplementary Figure S1 Spatiotemporal variations of key meteorological factors in the Pearl River Basin from 2000 to 2020. (a) Precipitation (Pre); (b) Minimum Temperature (Tmin); (c) Potential Evapotranspiration (PET); (d) Maximum Temperature (Tmax).

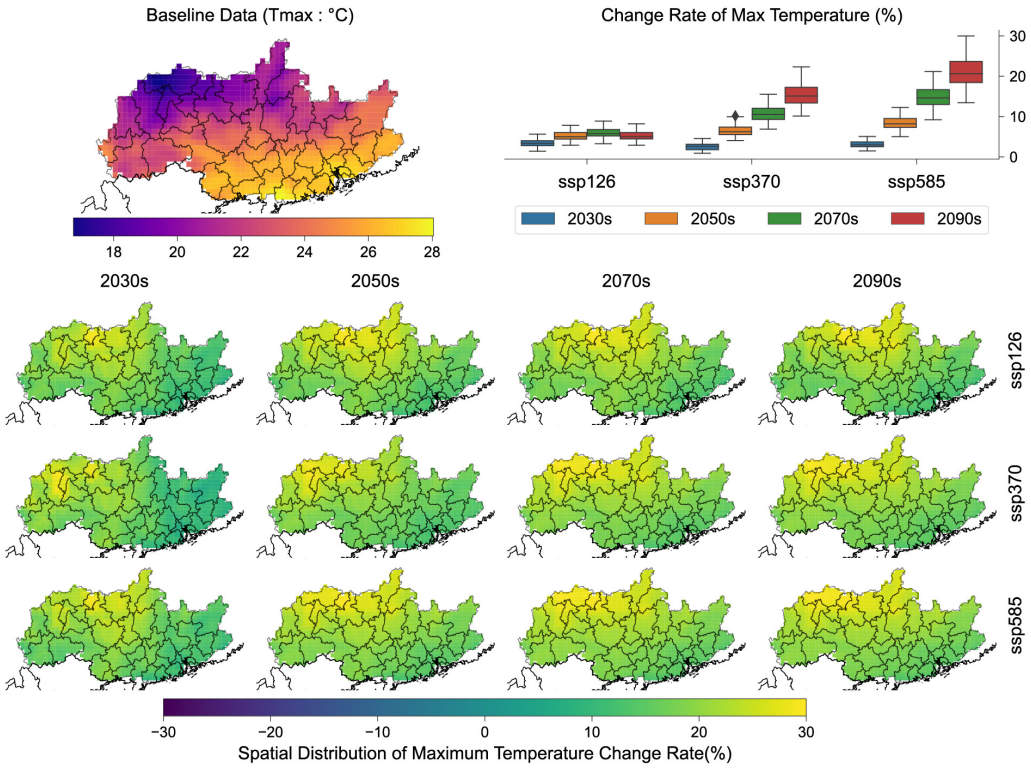
The color scales on the right of each map denote the range of each meteorological factor, while the profiles on the left and bottom of each map show the temporal changes in these factors across different latitudes and longitudes. The data indicates a clear trend of increasing temperature and potential evapotranspiration, along with significant spatial variability in precipitation patterns.



Supplementary Figure S2 Multi-year average sowing area and yield proportion by city.

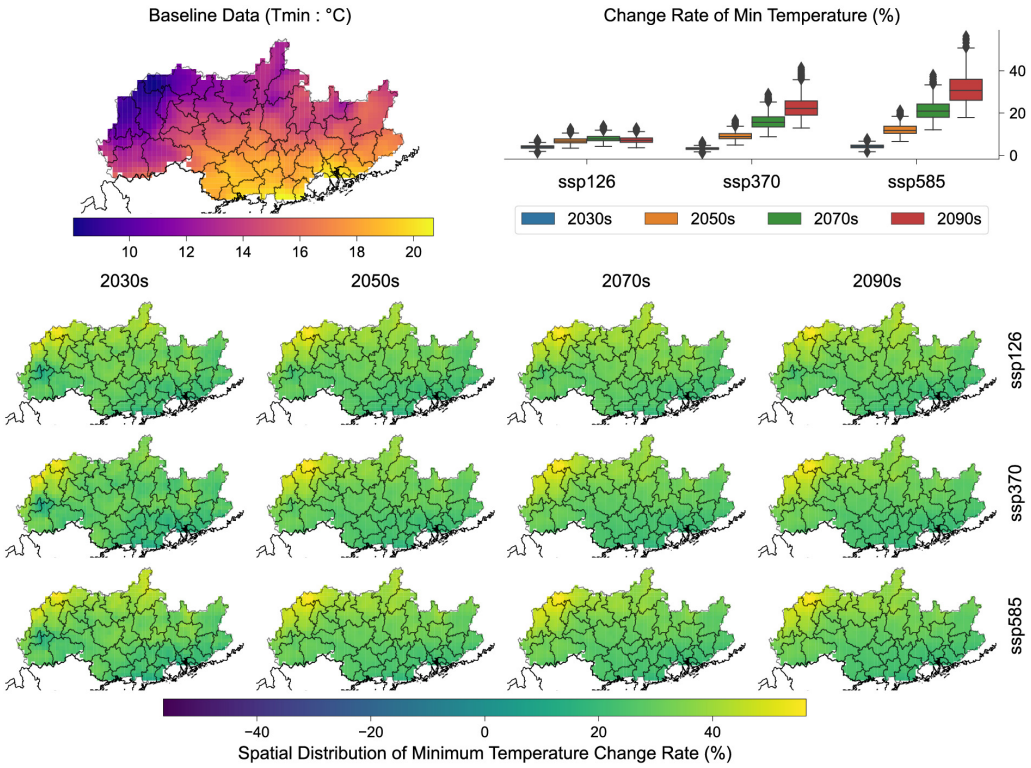


Supplementary Figure S3 First-order and total-order sensitivity indices for different crops.



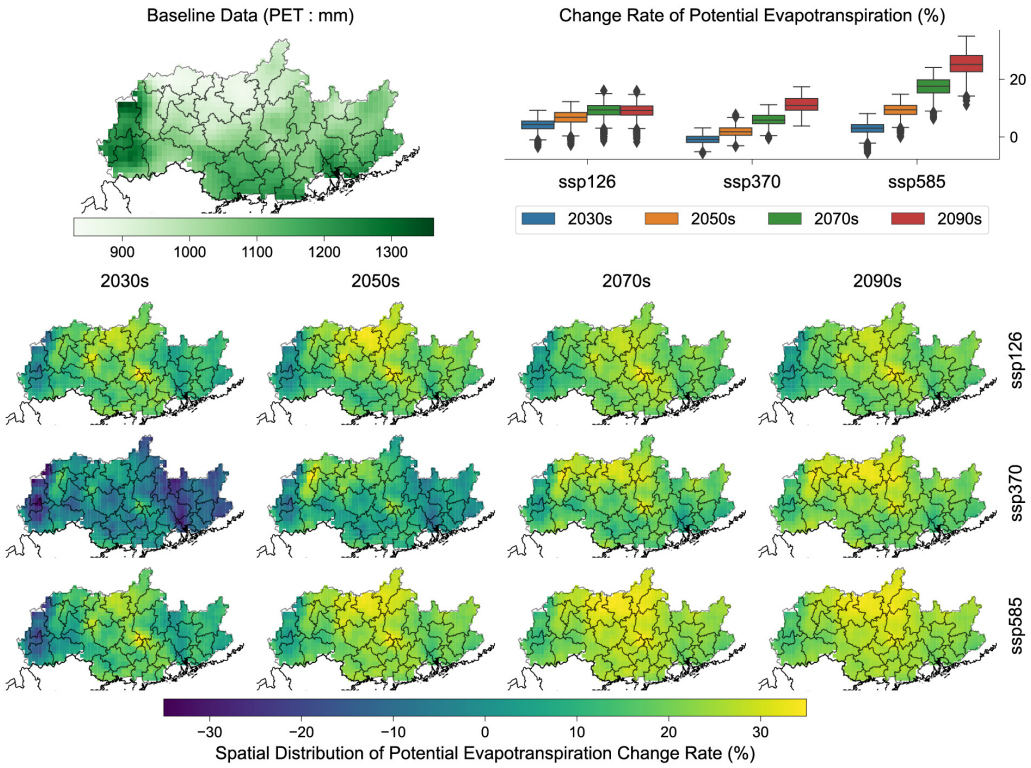
Supplementary Figure S4 Baseline maximum temperature and projected change rates under different SSP scenarios.

This figure illustrates the baseline Maximum Temperature data and the projected change rates of Maximum Temperature in the Pearl River Basin under three Shared Socioeconomic Pathways (SSPs) scenarios: SSP126, SSP370, and SSP585, across four future time periods (2030s, 2050s, 2070s, and 2090s). The periods are defined as same as precipitation.



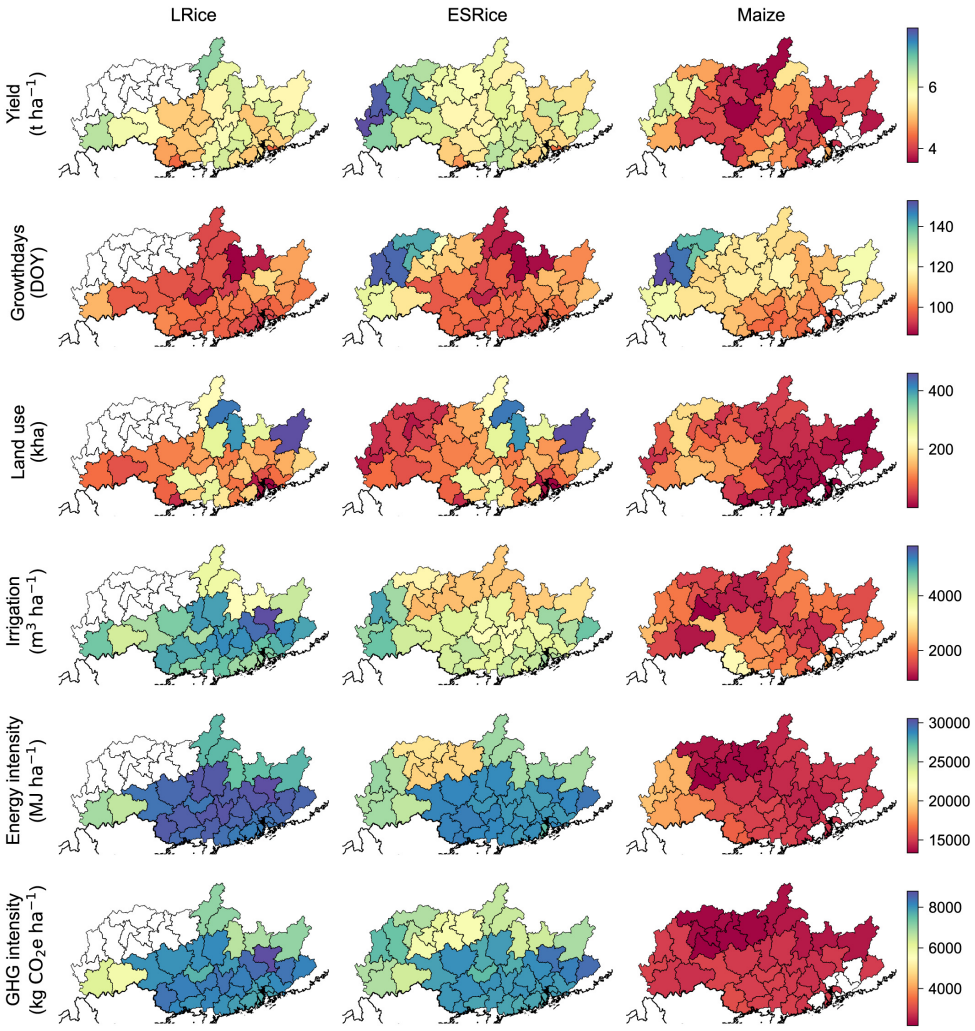
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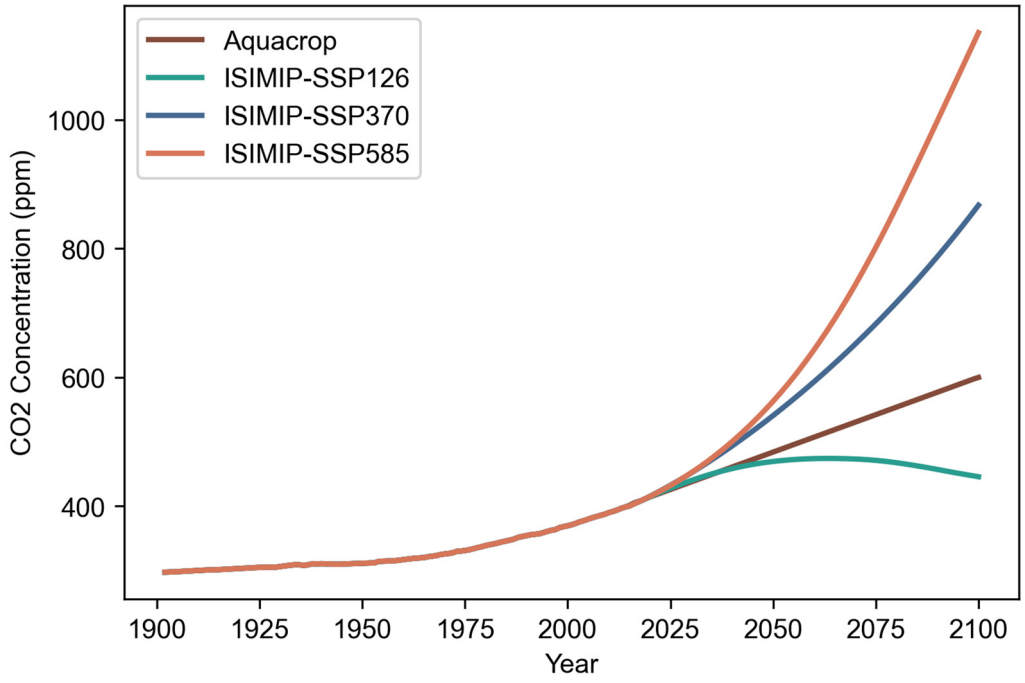
Supplementary Figure S6 Baseline potential evapotranspiration and projected change rates under different SSP scenarios.

This figure illustrates the baseline Potential Evapotranspiration data and the projected change rates of Potential Evapotranspiration in the Pearl River Basin under three Shared Socioeconomic Pathways (SSPs) scenarios: SSP126, SSP370, and SSP585, across four future time periods (2030s, 2050s, 2070s, and 2090s). The periods are defined as same as precipitation.

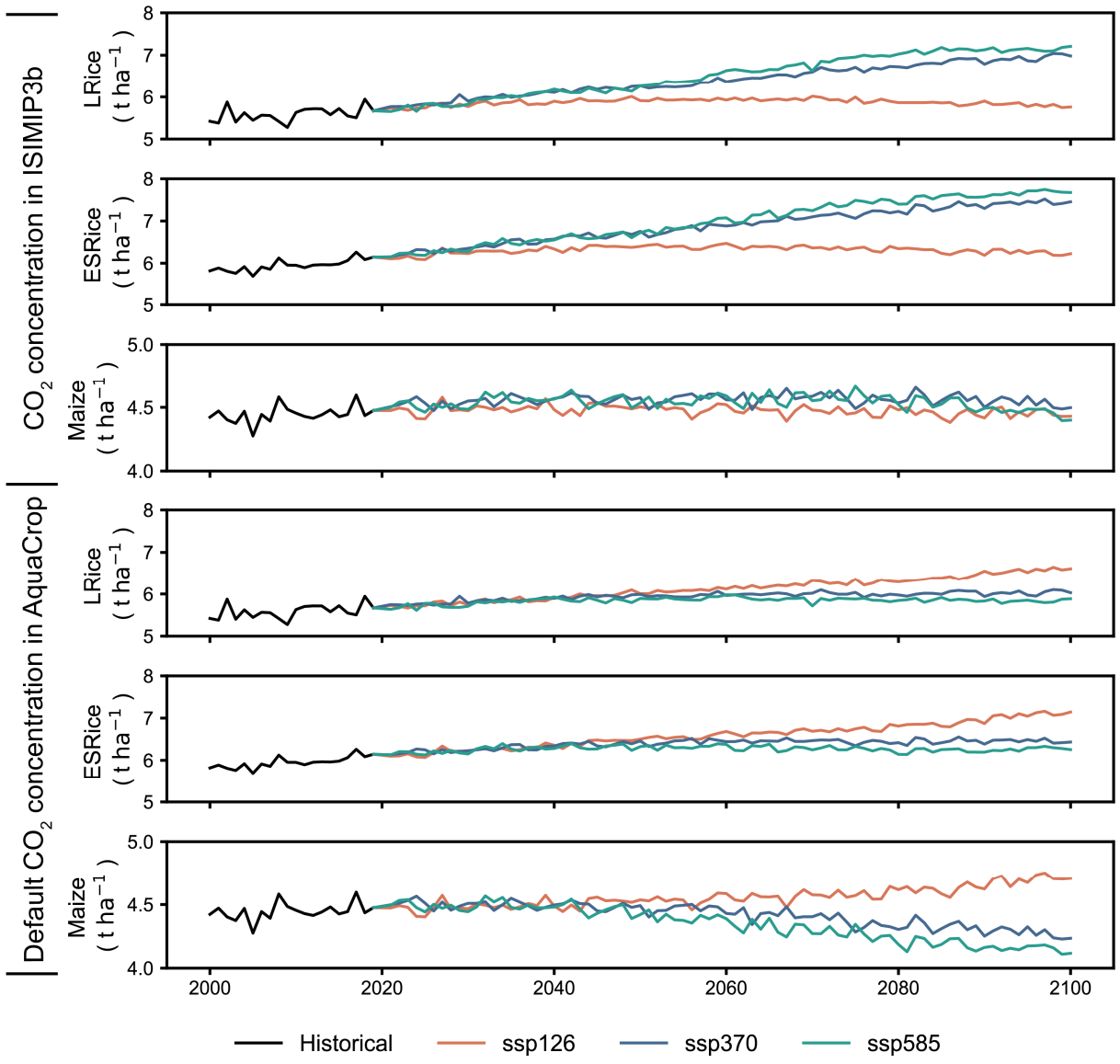


Supplementary Figure S7 WEFC-nexus of rice and maize in the Pearl River Basin during the 2010s.

This figure illustrates the Water-Energy-Food-Carbon (WEFC) nexus for three crops—late rice (LRice), early-single rice (ESRice), and maize—across different cities in the Pearl River Basin during the 2010s (2000-2020). Each row of maps represents one parameter, while each column represents a different crop (LRice, ESRice, and maize). The color bars on the right side of the maps indicate the range of values for each parameter.

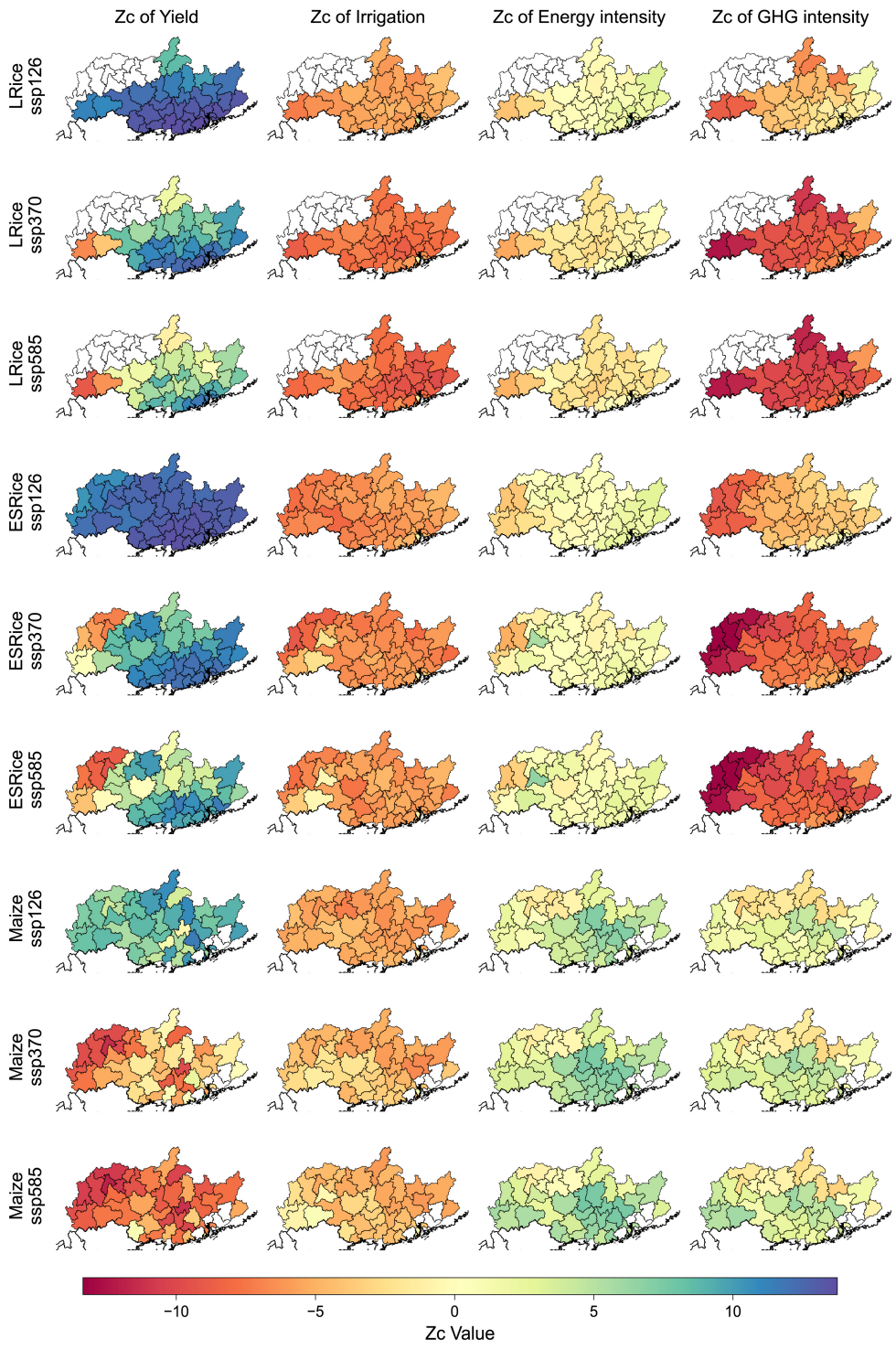


Supplementary Figure S8 CO_2 concentration over years for different models.



Supplementary Figure S9 Projected crop yields under different CO_2 concentration scenarios in ISIMIP3b and AquaCrop models.

This figure shows the projected crop yields of late rice (LRice), early-single rice (ESRice), and maize under different CO_2 concentration scenarios from the ISIMIP3b dataset and the default CO_2 concentration in the AquaCrop model from 2000 to 2100. The scenarios include historical data and three Shared Socioeconomic Pathways (SSPs): SSP126, SSP370, and SSP585.



Supplementary Figure S10 Spatial distribution of WEFC nexus trends for three crops under different SSP scenarios (based on default CO_2 concentration in the AquaCrop)

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