## Supplemental Figures:

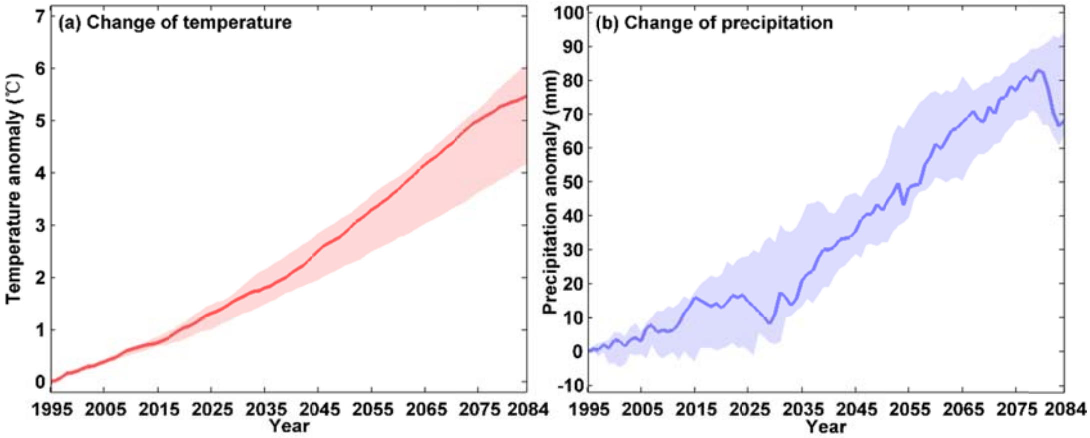


Figure S1 Change of (a) temperature and (b) precipitation from 1995-2084 with respect to 1981-2010 in the Yellow River (YR) basin under the RCP 8.5 emission scenario. The red (blue) shaded area denotes the interquartile range for the temperature (precipitation) anomaly and the solid line shows the median of the GCMs.

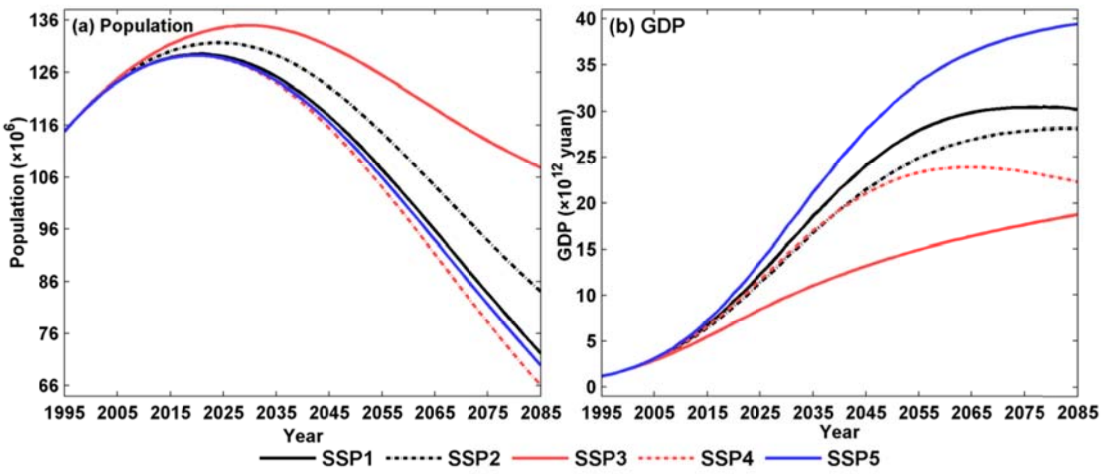


Figure S2 Population and gross domestic gross (GDP) from 1995-2085 in the Yellow River (YR) basin under SSP1, SSP2, SSP3, SSP4 and SSP5.

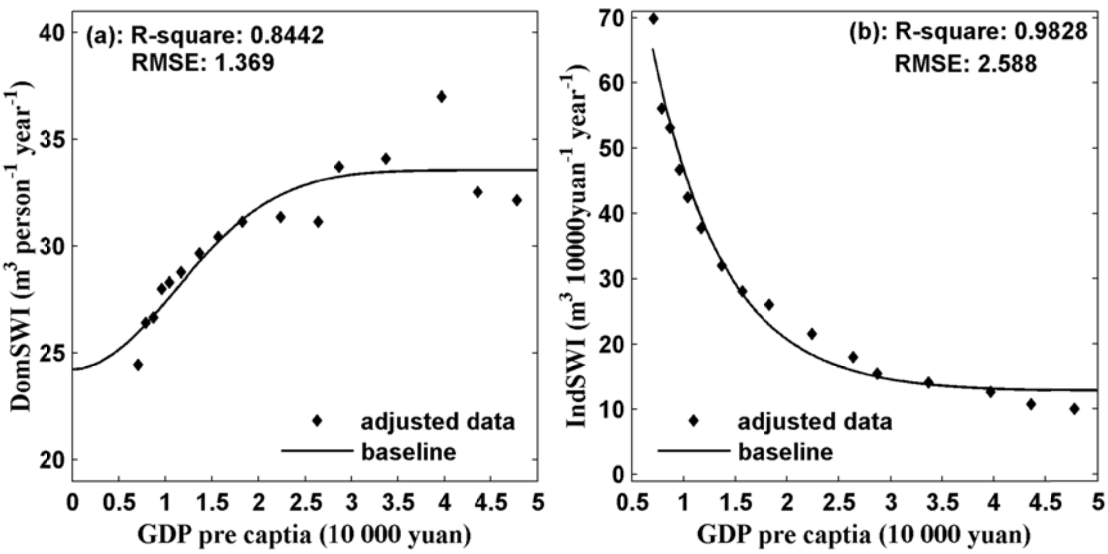


Figure S3 Structural changes in domestic water use intensity (DomSWI) (a) and industry water use intensity (IndSWI) (b) for the Yellow River (YR) basin.

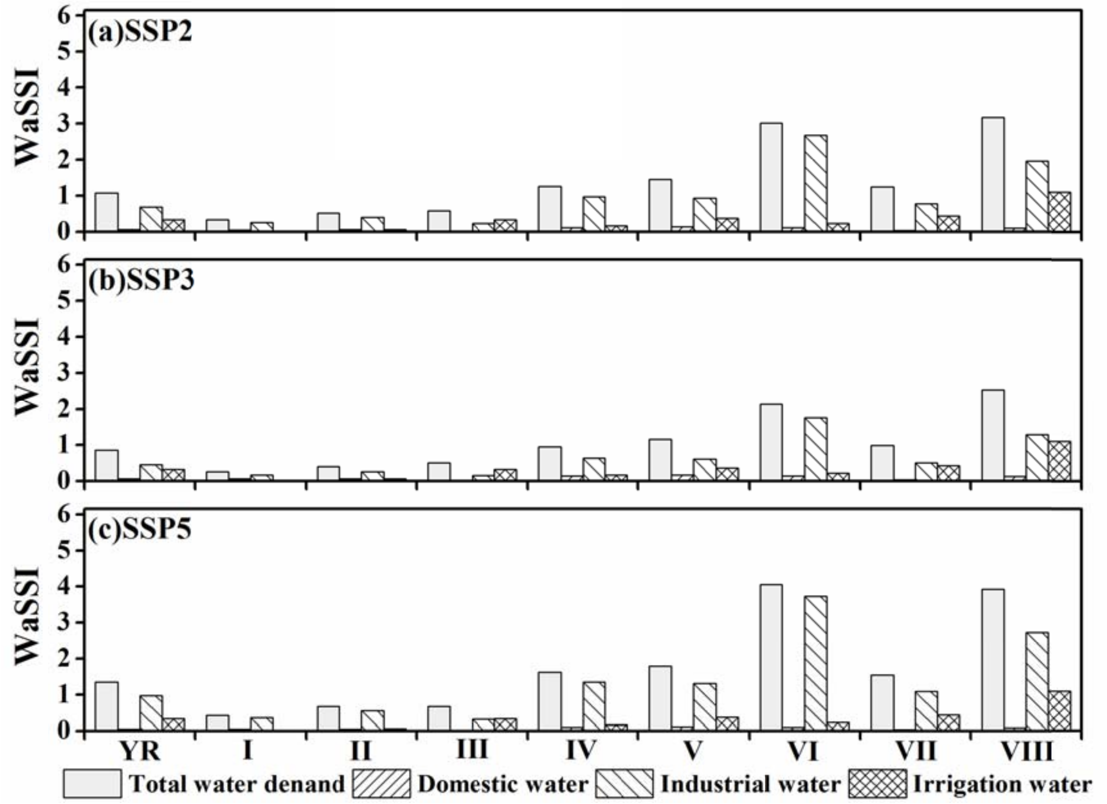


Figure S4 WaSSI for total water demand and for sectoral (domestic, industrial and irrigation) water demands for the Yellow River (YR) basin and eight sub-basins at the end of the 21st century under three different Shared Socio-Economic Pathways (SSPs) under RHWA70.

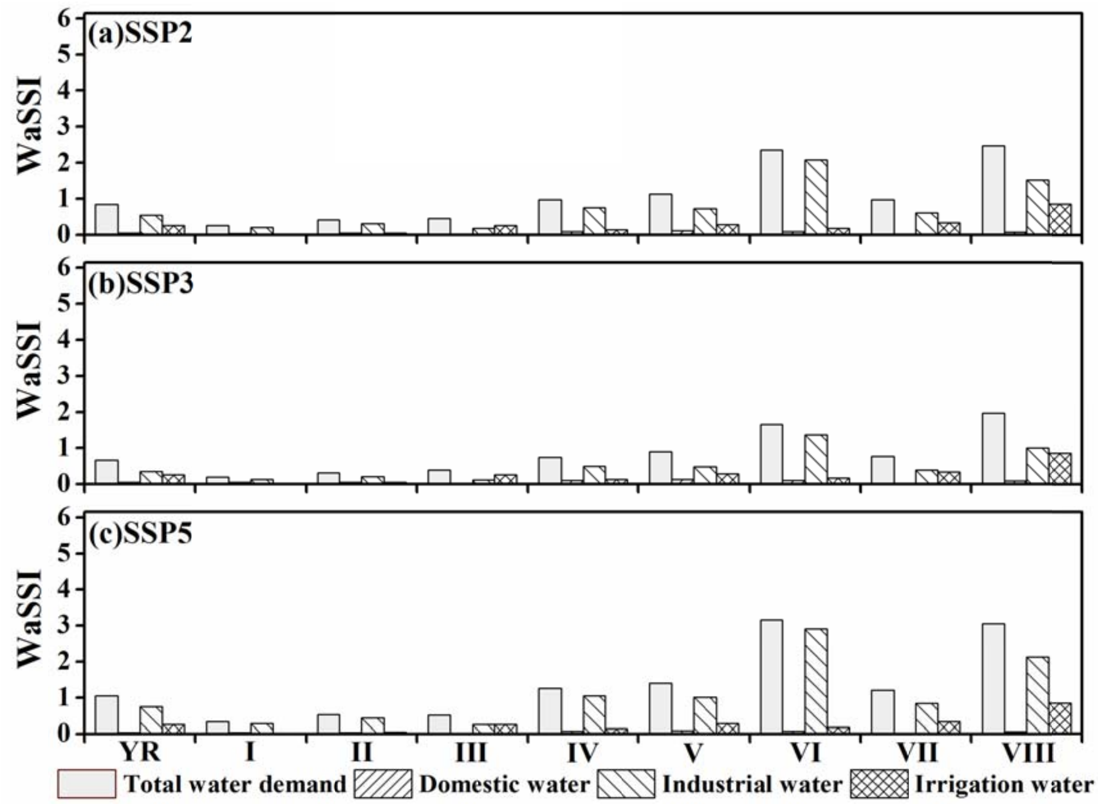


Figure S5 WaSSI for total water demand and for sectoral (domestic, industrial and irrigation) water demands for the Yellow River (YR) basin and eight sub-basins at the end of the 21st century under three different Shared Socio-Economic Pathways (SSPs) under RHWA90.

## Supplemental Tables:

Table S1 Main characteristics of the global gridded hydrological models (GGHMs) used in this study.

| Model name | Meteorological forcing[a] | Energy balance | Evaporation scheme[b] | Runoff scheme[c] | Snow scheme | Vegetation dynamics | $CO_2$ effect[d] | References |
|---|---|---|---|---|---|---|---|---|
| H80 | R, S, T, W, Q, LW, SW, SP | Yes | Bulk formula | Saturation excess, no-linear | Energy balance | No | No | Hanasaki et al. (200a, 2008b) |
| MPI-HM | P, T, W, Q, $LW_n$, SW, SP | No | Penman-Monteith | Saturation excess, no-linear | Degree Day | No | No | Hagemann et al. (2003); Stacke et al. (2012) |
| PCR-GLBWB | P, T | No | Hamon | Saturation excess, Beta function | Degree Day | No | No | Wada et al. (2010); Van Beek et al (2001); Wada et al. (2011) |
| VIC | P, T, W, Q, LW, SW, SP | Only for snow | Penman-Monteith | Saturation excess, no-linear | Energy balance | No | No | Liang et al. (1994); Lohmann and Raschke (1988) |
| WaterGAP | P, T, $LW_n$, SW | No | Priestley-Taylor | Beta function | Degree Day | No | No | Döll et al. (2012); Flörke et al. (2013) |
| WBM | P, T | No | Hamon | Saturation excess | Empirical temp and precip based formula | No | No | Vörösmarty et al. (1998); Wisser et al. (2010) |

Note: a R: rainfall rate, S: snowfall rate, P: precipitation rate (rain and snow calculated in the model), T: air temperature, W: wind speed, Q: air specific humidity, LW: downwellinglongwave

radiation; LWn: net longwave radiation; SW: downwelling shortwave radiation, SP: surface pressure.

b Bulk formula: Bulk transfer coefficients are used when calculating turbulent heat fluxes.

c Non-linear: Subsurface runoff is a non-linear function of soil moisture.

d $CO_2$ concentration in calculation of stomatal conductance.

Table S2 Main characteristics of the global gridded crop models (GGCMs) used in this study.

| Model name | Meteorological forcing [a] | Evapo-transpiration | Stresses [b] | $CO_2$ effect [c] | Yield function [d] | Institution | References |
|---|---|---|---|---|---|---|---|
| EPIC | Tmn, Tmx, P, Rad, RH, WS | Penman-Monteith | W, T, H, A, N, P, BD, Al | RUE, TE | $HI_{WS}$, PrtB | BOKU, University of Natural Resources and Life Sciences, Vienna | Williams (1995); Izaurralde et al. (2006) |
| GEPIC | Tmn, Tmx, P, Rad, RH, WS | Penman-Monteith | W, T, H, A, N, P, BD, Al | RUE, TE | $HI_{WS}$, PrtB | EAWAG, Swiss Federal Institute of Aquatic Science and Technology | Williams (1990); Liu et al. (2007) |
| LPJmL | Ta, P, Cld (or Rad) | Priestley-Taylor | W, T | LF, SC | $HI_{WS}$ | Potsdam Institute for Climate Impact Research | Bondeau et al. (2007); Fader et al. (2010) |
| LPJ-GUESS | Ta, P, Cld (or Rad) | Priestley-Taylor | W, T | LF, SC | $HI_{WS}$ | Lund University, Department for Physical Geography and Ecosystem Science, IMK-IFU, Karlsruhe Institute of Technology, Garmisch-Partenkirchen, Germany | Bondeau et al. (2007); Smith et al. (2011) |
| pDSSAT | Tmn, Tmx, P, Rad | Priestley-Taylor | W, T, H, A, N | RUE (for wheat, rice, maize) and LF (for soybean) | Gn | University of Chicago Computation Institute | Elliott et al. (2014); Jones et al. (2013) |
| PEGASUS | Ta, Tmn, Tmx, P, Cld (or Sun) | Priestley-Taylor | W, T, H, N, P, K | RUE | Prt | Tyndall Centre University of East Anglia, UK/McGill University, Canada | Deryng et al. (2011) |

Note: a Tmn: Minimum temperature, Tmx: Maximum temperature, P: Precipitation, Rad: Percentage of radiation, RH: Relative humidity, WS: Wind speed, Ta: Average temperature, Cld: Percentage of cloud cover, Sun: Fraction of sunshine hours

b W: water stress; T: temperature stress; H: specific-heat stress; A: oxygen stress; N: nitrogen stress; P: phosphorus stress; K: potassium stress; BD: bulk density; Al: aluminum stress (based on pH and base saturation)

c Elevated $CO_2$ effects: LF: Leaf-level photosynthesis (via rubisco or quantum-efficiency and leaf photosynthesis saturation; RUE: Radiation-use efficiency; TE: Transpiration efficiency; SC: stomatal conductance

d Yield formation depending on: HI: Fixed harvest-index; HIws: HI modified by water stress; Prt: Partitioning during reproductive stages; B: Total (above-ground) biomass; Gn: Number of grains and grain growth rate

Table S3 Overview of global climate models (GCMs) used in this study.

| | Name | Institute | References |
|---|---|---|---|
| GCMs | HadGEM2-ES | Met Office Hadley Centre | Jones et al. (2011) |
| | IPSL-CM5A-LR | Institute Pierre-Simon Laplace | Mignot et al. (2013) |
| | MIROC-ESM-CHEM | Japan Agency for Marine-Earth Science and Technology, Atmosphere and Ocean Research Institute (The University of Tokyo), and National Institute for Environmental Studies | Watanabe et al. (2011) |
| | GFDL-ESM2M | Geophysical Fluid Dynamics Laboratory | Dunne et al. (2012, 2013) |
| | NorESM1-M | Norwegian Climate Centre | Bentsen et al. (2013); Iversen et al. (2013) |

Table S4 Comparisons of average annual runoff between the observations and estimates of seven GGHMs at the selected hydrological stations during 1971-2000 in billion $m^3$ per year.

| Hydrological stations | Lanzhou | Longmen | Sanmenxia | Huayuankou |
|---|---|---|---|---|
| Observation | 32.74 | 37.59 | 47.81 | 53.04 |
| GGHM-GCMs | 38.9 | 47.32 | 64.41 | 68.79 |
| H08 | 49.11 | 59.24 | 78.17 | 82.17 |
| MPI-HM | 12.26 | 14.3 | 25.18 | 28.21 |
| PCR-GLOBWB | 63.25 | 82.12 | 117.38 | 125.74 |
| VIC | 44.58 | 64.51 | 92.52 | 98.48 |
| WaterGAP | 25.61 | 33.36 | 47.67 | 51.41 |
| WBM | 34.66 | 37.03 | 44.72 | 45.55 |

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