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Estimation of Watershed Hydrochemical Responses to Future Climate Changes Based on CMIP6 Scenarios in the Tianhe River (China)

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1. Chosen of GCMs

There are seven GCMs considered, which are detailed descripted in Table S1. The climate change estimation based on CMIP6 is a work in progress and the outputs of different GCMs are constantly being published. These seven GCMs have whole outputs for the four periods and four SSP scenarios and have been downscaled for 2.5 minutes resolution and are available at WorldClim dataset. Although more complete estimations can be attached after all GCMs finished, the purpose of this study now is to provide a quick perspective based on the existing GCMs outputs to estimate the impacts of climate changes on watershed under CMIP6 scenarios.

Table S1. Descriptions of GCM models used in this study.

GCM	Research centre	Nominal resolution
BCC-CSM2-MR	The Beijing Climate Center Climate System Model	100km
CNRM-CM6-1	the National Center for Meteorological Research, Météo-France and CNRS laboratory (CNRM/CERFACS)	250km
CNRM-ESM2-1	the National Center for Meteorological Research, Météo-France and CNRS laboratory (CNRM/CERFACS)	250km
CanESM5	The Canadian Centre for Climate Modelling and Analysis	500km
IPSL-CM6A-LR	The Institut Pierre - Simon Laplace	100km
MIROC-ES2L	the Model for Interdisciplinary Research on Climate, Earth System version 2 for Long-term simulations	500km
MIROC6	the Model for Interdisciplinary Research on Climate	100km

2. Applications of LARS-WG

The LARS-WG was firstly calibrated based on 63 years of observed daily weather data in the study area. The model parameters can be found in the Supplementary Material folder as a text file named "XunXi.wgx", which can be to reproduce the results. Then, based on the calibrated parameters, the LARS-WG model was operated and 63 years of synthetic daily weather data were generated and compared with the observed data to validate the parameters, the results of which is provided in the Supplementary Material folder as a text file named "XunXi.tst". The random seed number of 3767 is used to generate synthetic weather series. The model can be considered reliable if the statistical distribution characteristics of the modelled values and the observed values are consistent with no significant difference at the 5% significance level.

The calibrated and validated LARS-WG model can generate any lengths of synthetic daily weather data that present the current climate status in the study area. The synthetic daily weather data presenting future climate status can also be generated using LARS-WG just needing to update the model parameters based on scenario files, which are provided as a series of text files in the subfolder of the Supplementary Materia named "Scenario Files of CMIP6 for LARS-WG". These scenario files can be used to reproduce the scenario analysis results of LARS-WG. For each scenario file, groups of variable changes for each month need to be provided, including the relative change in monthly mean rainfall, absolute changes in monthly mean min temperature, and absolute changes in monthly mean max temperature. The data in scenario files are calculated based on the average of seven GCMs outputs as the ensemble. For each GCM, the scenario analysis results in the study area are obtained using a Python batch procedure developed for site value extraction based on the data format of Worldclim, which can be found in the subfolder of the Supplementary Materia named "Python batch procedure". More details about Python file setup can be found in the annotation in the file of "DataExtraction.py". With the updated parameters, twenty years of synthetic daily weather data were generated for each SSP scenario and future period, which can be found in the subfolder of the Supplementary Materia named "Synthetic Weather Series of LARS-WG". These synthetic weather data can be used to reproduce the scenario analysis results of ReNuMa.

3. Applications of ReNuMa

The model parameters of ReNuMa used in this study are listed in Table S2 and Table S3, which can be used to reproduce the work.

Table S2. Hydrological Parameters of Regional Nutrient Management (ReNuMa) model.

Parameter Items.	Subcategories	Parameter Values
runoff curve number	Paddy fields	97.22
	Cultivated land	89.59
	Wood land	61.04
	Shrubbery lands	78.18
	Sparsely forested woodland	84.96
	Other forest land including garden	77.97
	High coverage grassland	77.22
	Middle coverage grassland	78.47
	Low coverage grassland	86.16
	Water surface	82.58
	Cities and towns	100.00
	Rural residential land	98.44
et cover factor	JAN	0.50
	FEB	0.50
	MAR	0.70
	APR	0.70
	MAY	0.70
	JUNE	0.70
	JULY	0.70
	AUG	0.70
	SEPT	0.70
	OCT	0.50
	NOV	0.50
	DEC	0.50
Groundwater flow	Quick recession coefficient	0.0156
	Quick seepage coefficient	0.0141

Parameter Items.	Subcategories	Parameter Values
	Slow recession coefficient	0.0085
	Slow seepage coefficient	0.0000
	Ground Water Limite for recession (cm)	5.00
	Ground Water Limite for seepage (cm)	5.00
	Unsat Avail Wat(cm)	6.07
	Unsat leakage coefficient	0.0931

Table S3. Nutrient Parameters of Regional Nutrient Management (ReNuMa) model.

Parameter Items	Subcategories	Parameter Values
Deposition	Annual atmosphere nitrogen depositions (kg/ha/year)	11.18
	Dry nitrogen deposition fraction	0.5
Septic systems	Population served by normal septic systems	74598
	Per capita tank nitrogen effluent (g/day)	6.0
	per capita grow season nitrogen uptake (g/day)	1.6
NANI Parameters	Agriculture class runoff nitrogen concentration intercept	1.5000
	Agriculture class runoff nitrogen concentration slope	0.0100
	Agriculture class runoff nitrogen concentration slope increment	0.1000
	Agriculture class runoff nitrogen concentration threshold	130.00
	Forest class runoff nitrogen concentration intercept	0.0140
	Forest class runoff nitrogen concentration slope	0.0000
	Forest class runoff nitrogen concentration slope increment	0.2000
	Forest class runoff nitrogen concentration threshold	10.000

4. Algorithms

4.1. Nash-Sutcliff coefficient

The Nash-Sutcliff coefficient and linear coefficient of determination, referred to as R^2_{NS} and r^2 respectively, were used as the test statistic. The R^2_{NS} can be formulated as:

$$R_{NS}^2 = 1 - \frac{\sum_{i=1}^{n}(O_i - P_i)^2}{\sum_{i=1}^{n}(O_i - \bar{O})^2}$$

In which O_i indicates the observed value, P_i the modeled value, $\bar{O}$ indicates the mean value of all observed values. For the R^2_{NS}, among its logical range from minus infinity to 1, it is a measure of the prediction accuracy, with the value 1 indicating a perfect fit. A value of R^2_{NS} less than zero implies that the model predicted values are less accurate than simply using the observed mean. The Nash-Sutcliffe statistic mainly concerns the sum of squared deviations from predicted values versus observed datasets was and is widely used in model calibration, but it is likely to be more sensitive to large values due to their relative weight in achieving an optimal goodness-of-fit. However, considering both R^2_{NS} and r^2 statistics in combination can provide a reasonable view of assessing the capability of the model to fit the data.

4.2. Additional algorithm of segment function in ReNuMa

The segment function was introduced to characterize daily recession and seepage in ReNuMa. The groundwater transfer coefficients here were divided into quick and slow recession and seepage coefficients depending upon whether the saturated zone water storage was above or below a threshold value, which can be formulated as:

$$\text{Daily recession coefficient} = \begin{cases} \text{recession coefficient}_{\text{quick}}(\text{saturated zone storage} \geq \text{threshold}_{\text{recession}}) \\ \text{recession coefficient}_{\text{slow}}(\text{saturated zone storage} < \text{threshold}_{\text{recession}}) \end{cases}$$

$$\text{Daily seepage coefficient} = \begin{cases} \text{seepage } coefficient_{quick}\left(saturated\ zone\ storage \geq threshold_{\text{seepage}}\right) \\ \text{seepage } coefficient_{slow}\left(saturated\ zone\ storage < threshold_{\text{seepage}}\right) \end{cases}$$

In this algorithm, two groups of groundwater transfer coefficient were used in the model. When the saturated zone water storage is smaller than a threshold value (a low-flow situation), the slow transfer coefficients would be applied to calculate the slow transfer process on that day. Otherwise, the quick flow coefficients would be used to represent the normal groundwater process. The critical threshold parameter for saturated zone storage is obtained by calibration.