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A coupled surface water-groundwater multi-objective optimization framework for coordinated water-ecosystem-agriculture management in arid inland river basin

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S1 Data sources and preprocessing

This section provides detailed information on the datasets used in this study, including their sources, spatial and temporal resolutions, and specific applications, supplementing the brief description in Section 2.2 (Data).

The datasets employed in this study primarily include meteorological forcing data, remote sensing products, hydrological observations, and model validation data. Surface runoff and snowmelt runoff data were obtained from the GLDAS-2.1 Noah model product, spatially downscaled to a 2 km × 2 km resolution, and further aggregated to daily values to drive the GSFLOW model. Meteorological variables, including precipitation, daily maximum temperature, and daily minimum temperature, were derived from the ERA5 reanalysis dataset and similarly downscaled for use as model inputs.

GRACE data were obtained from the RL06 Mascon Level-3 product released by the Center for Space Research (CSR) at the University of Texas at Austin, covering the period from April 2002 to December 2021. Missing monthly values were filled using cubic spline interpolation. For the gap between the GRACE and GRACE-FO missions (July 2017 to May 2018), terrestrial water storage reconstruction data developed by Zhong et al. (2019, 2020) were used to ensure a continuous time series. Monthly terrestrial water storage change (TWSC) was calculated from the TWSA series as follows:

$$\mathrm{TWSC}(t) = \mathrm{TWSA}(t) - \mathrm{TWSA}(t-1)$$

where TWSC(t) represents the change in terrestrial water storage (mm) during month t, and TWSA(t) represents the corresponding storage anomaly.

Detailed information on the spatial and temporal resolutions of these datasets and their specific applications is provided in Supplementary Table S1.

Table S1. Data for the coupled hydrology-agriculture optimization framework.

Data	Dataset / Source	Spatial & Temporal Resolution	Usage
Snow cover	High Asia MODIS daily snow cover fraction dataset	500 m| Daily	Model input
Climate forcing	ERA5 reanalysis	0.25°×0.25°| hourly	Model input
Topography	ASTER GDEM	30 m	Model input
Hydrogeology	hydrogeological maps, borehole data	Site-specific	Model input
Land surface	FROM-GLC, HWSD. Vegetation Map of China,	Dataset-specific	Model input
Socio-economic data	XSB, XWRB, NAPCBC & ARAX	Annual	Model input
Groundwater level	Monitoring wells	Monthly	Model validation
Terrestrial water storage changes	GRACE/GRACE-FO (CSR RL06 Mascon)	0.25°×0.25°| month	Model validation
Evapotranspiration	GLEAM	0.25°×0.25°| monthly	Model validation
Soil moisture	Soil Moisture in China dataset	0.05°×0.05°| monthly	Model validation

S2 Geological section map of model area

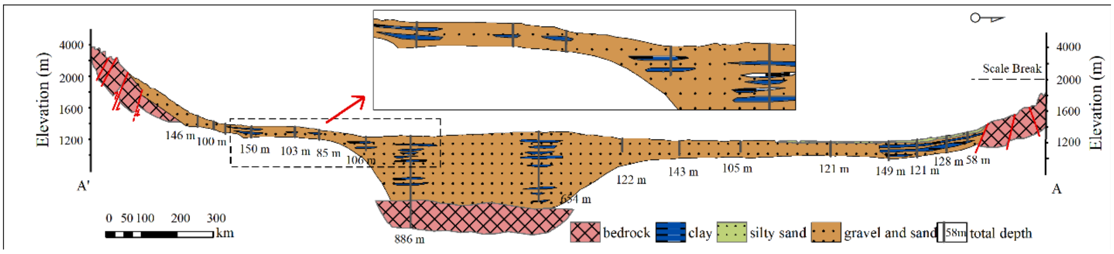

Figure S1. Geological section map of model area.

S3 Schematic diagram of model boundaries

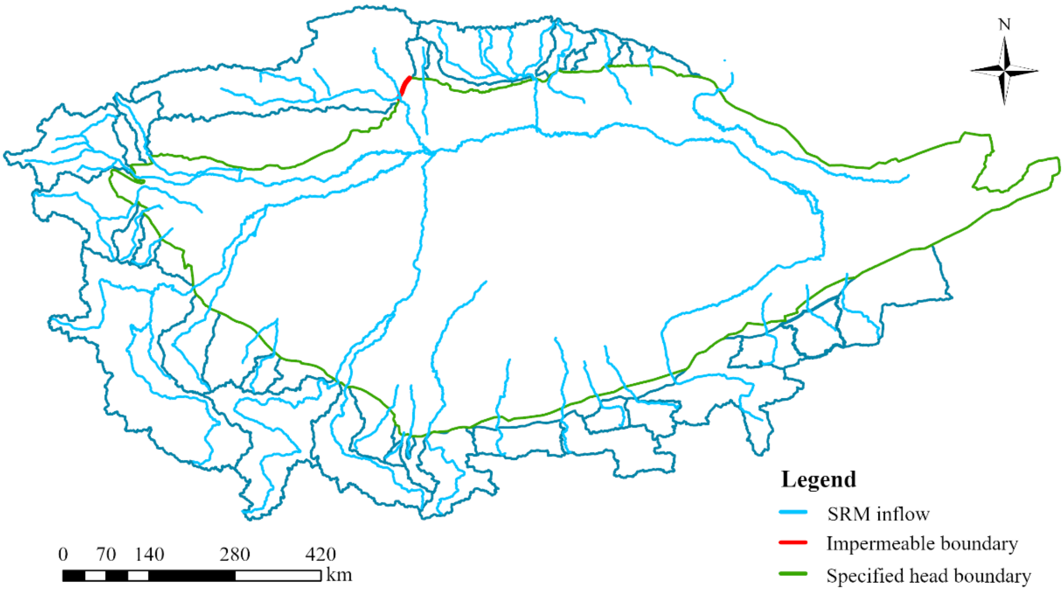

Figure S2. Schematic diagram of model boundaries.

S4 Evaluation of snowmelt runoff model's performance

The following results present the performance of the SRM model across the sub-catchments in the study area. The spatial distribution and numbering of the sub-catchments are shown in Figure S3.

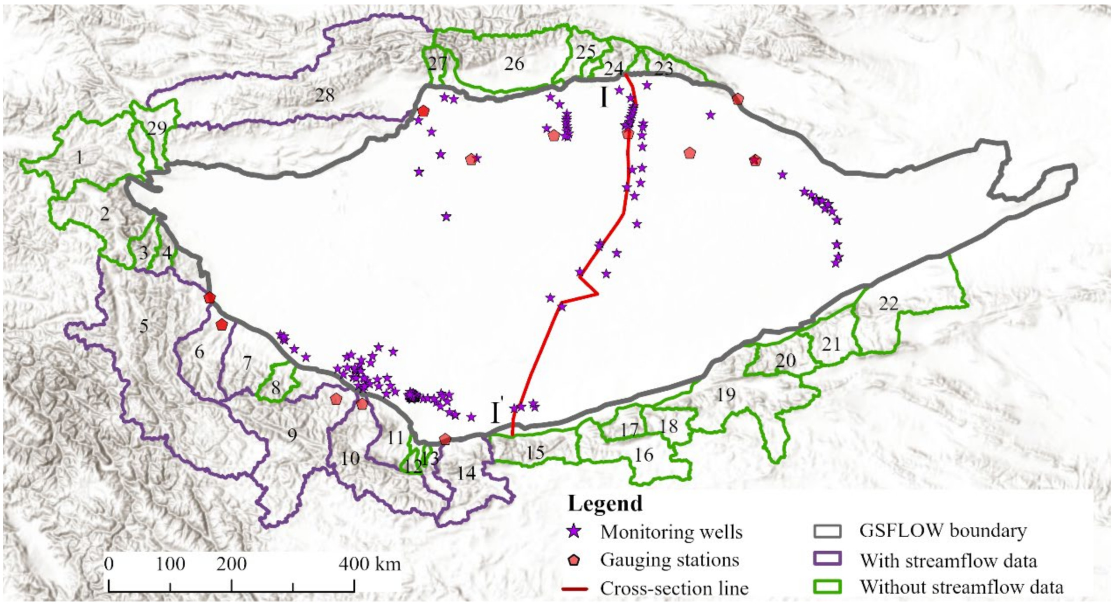

Figure S3. Spatial distribution and numbering of sub-basins in the study area. Sources: Esri; Powered by Esri; Basemap: Esri World 286 Hillshade (Esri).

For the catchments with observed streamflow data (i.e., No.5, No.6, No.9, No.10, No.14, and No.28), the calibration and validation results of the SRM model are summarized in Figure S4. The left column shows the time series of observed and simulated monthly streamflow during the calibration period (2002-2015) and the validation period (2016-2021), while the two columns on the right present scatter comparisons between modeled and observed runoff for the corresponding periods.

For the catchments without observed streamflow data (i.e., No.1, No.2, No.4, No.7, No.8, No.11, No.12, No.15, No.19, No.20, No.21, No.24, No.25, No.26, No.27, and No.29), SRM model parameters were derived from calibrated catchments using a hydrological similarity approach. Model performance was evaluated using multi-year mean streamflow series, and the results are shown in Figure S5.

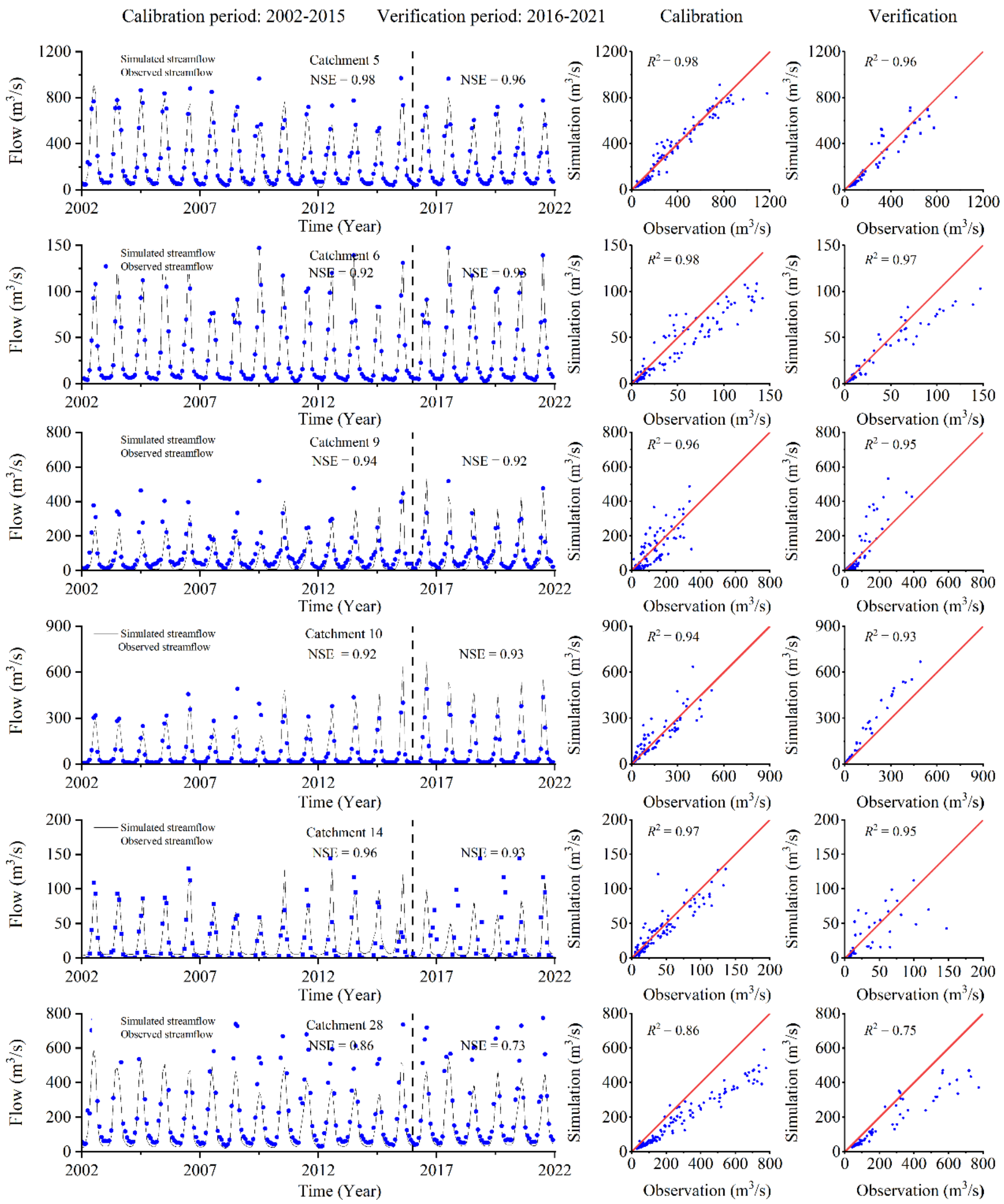

Figure S4. Observed and simulated monthly streamflow for catchments No.5, No.6, No.9, No.10, No.14, and No.28. The left column shows the time series of observed and simulated streamflow during the calibration (2002-2015) and validation (2016-2021) periods. The two right columns present scatter comparisons between observed and simulated monthly streamflow for the calibration and validation periods, respectively.

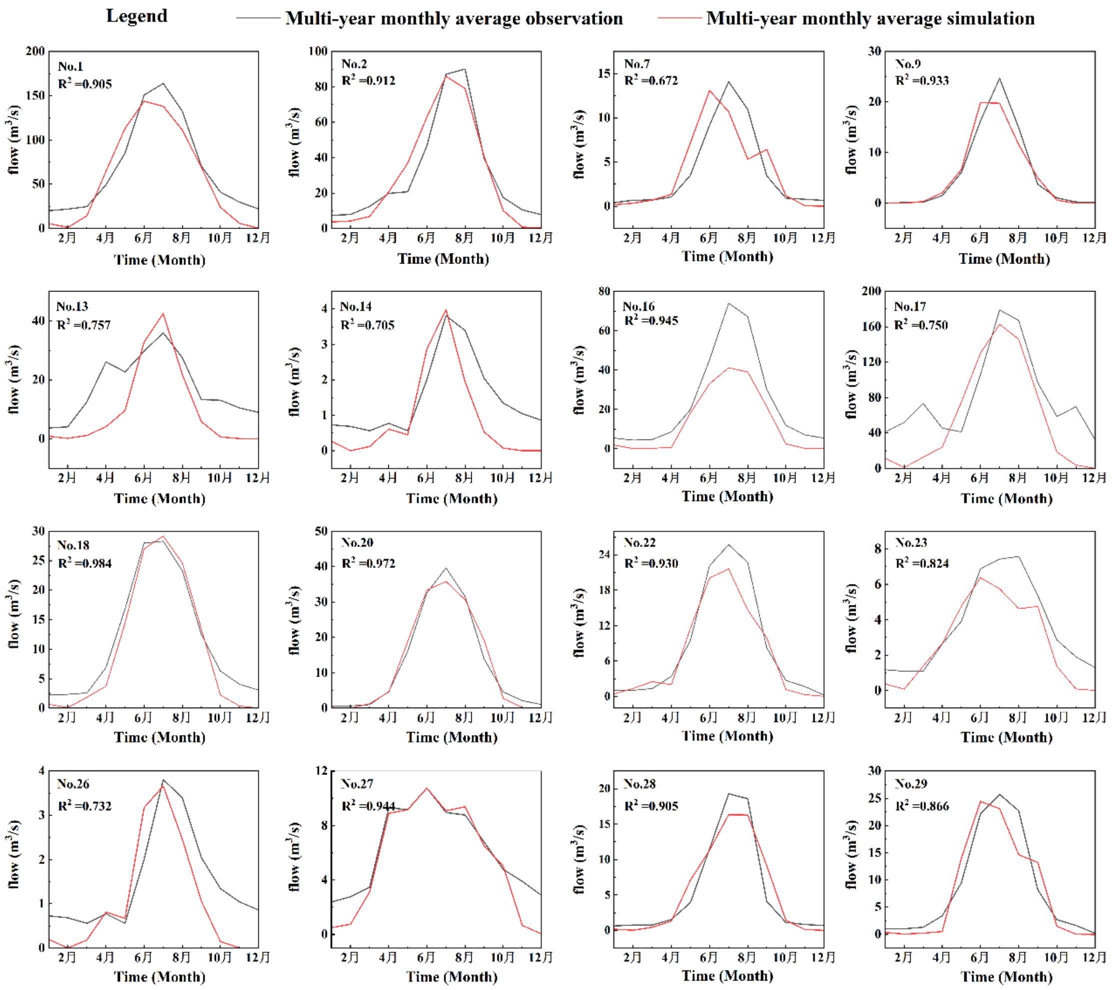

Figure S5. Comparison between simulated and observed multi-year mean streamflow for ungauged catchments, including No.1, No.2, No.4, No.7, No.8, No.11, No.12, No.15, No.19, No.20, No.21, No.24, No.25, No.26, No.27, and No.29.

S5 Evaluation of the surface water-groundwater model performance using remote sensing data

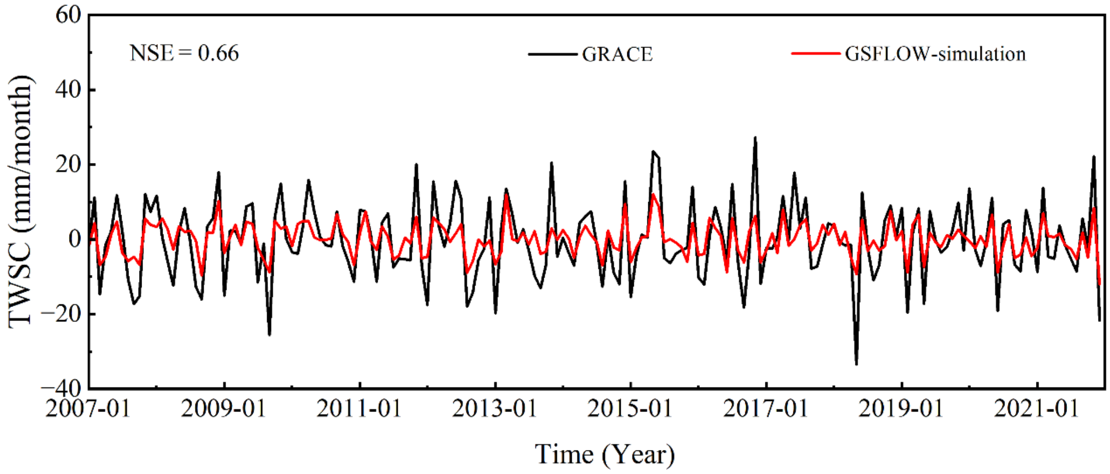

Figure S6. Comparison of monthly variations in total water storage change (TWSC) derived from the GSFLOW simulations and GRACE.

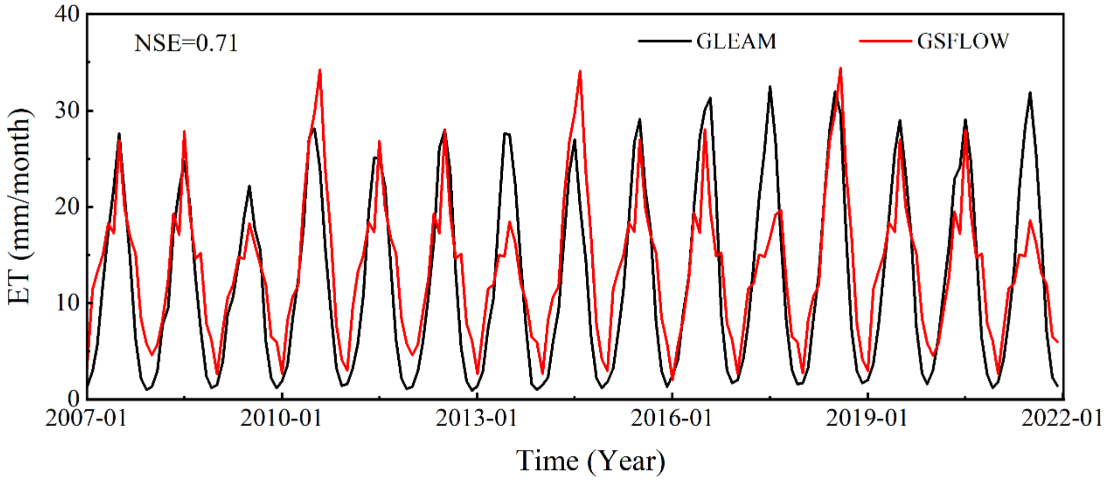

Figure S7. Evaluation of monthly evapotranspiration (ET) simulated by the GSFLOW model against GLEAM-based estimates for the period 2007-2021.

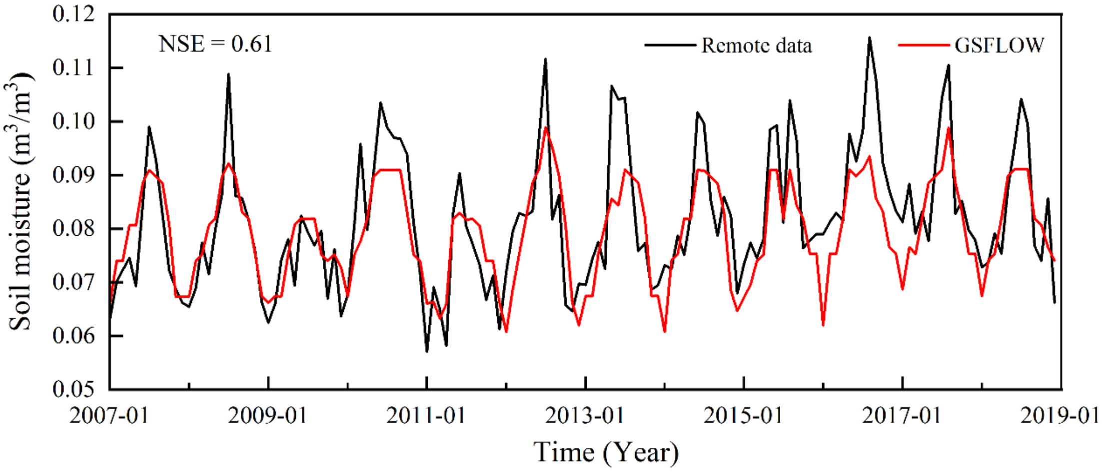

Figure S8. Comparison between GSFLOW-simulated and remotely sensed monthly soil moisture during 2007-2018.

S6 Evaluation of the surrogate model performance

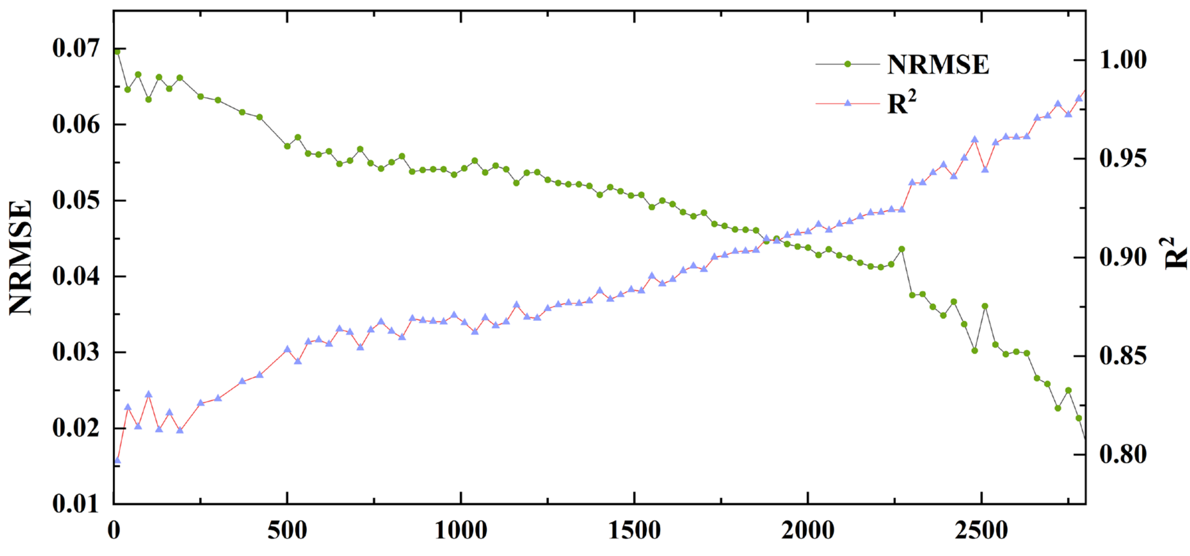

Figure S9. Variation of the surrogate model's NRMSE and R^2 with the number of training samples.

Table S2. Five-fold cross-validation results for the surrogate model

Target	Fold 1 RMSE	Fold 2 RMSE	Fold 3 RMSE	Fold 4 RMSE	Fold 5 RMSE	Mean RMSE	Std RMSE
Groundwater level	0.031	0.035	0.032	0.036	0.033	0.033	0.002
Lake area	1.012	1.124	1.036	1.146	1.058	1.075	0.057