



Integrating Fully-Coupled Hydrological Modeling and Random Forest to Enhance Spatial Resolution of GRACE-Observed Water Storage Across the Rhine Basin

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The gravity recovery and climate experiment (GRACE) satellite offers valuable data for hydrological analysis but its coarse spatial resolution limits its effectiveness for local-scale studies. While statistical downscaling techniques using global hydrological model outputs have shown promise in enhancing the resolution of terrestrial water storage (TWS) estimates from GRACE data, the performance of GRACE TWS downscaling based on regional fully-coupled model outputs remains unexplored. In this study, we analyzed to appraise the feasibility of GRACE TWS downscaling under two scenarios. The first scenario included training a machine learning algorithm with global hydrological (Famine Early Warning Systems Network (FEWS NET) Land Data Assimilation System (FLDAS)) model outputs. In the second scenario, ParFlow and CLM (PFC) models were combined in a fully surface–subsurface coupled modeling, and the outputs were integrated into a Random Forest machine learning downscaling technique. The downscaled TWS values (0.1°) were then evaluated against the GRACE TWS (0.25°) and precipitation observations of the rain gauges over the Rhine basin in Germany. The PFC-based downscaled TWS showed stronger correlation (0.98) than the FLDAS-based downscaled TWS (0.80). Comparison of the downscaled TWS results with precipitation data also emphasized the superiority of the second scenario. The PFC model-based downscaled TWS demonstrated increased correlations with precipitation data over all the sub-basins of the Rhine, suggesting that training downscaling algorithms with the fully-coupled physics-based hydrological model outputs yield better results compared to those of the FLDAS model.

KEY WORDS: GRACE, Terrestrial water storage, Machine learning, ParFlow-CLM, Downscaling, FLDAS.

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INTRODUCTION

Terrestrial water storage (TWS) is essential to the water cycle. It includes the cumulative amount of water stored vertically on or below the earth's surface, making it a vital factor in understanding and managing water resources (Youssefi et al., 2022; Humphrey et al., 2023). Satellite-based assessment of TWS fluctuations is a surrogate approach that has benefits compared to orthodox field-based moni-

toring techniques. The latter possess superior data quality; nevertheless, they are impeded by the scarcity of in situ observations, especially in large areas (Ali et al., 2021a, 2021b; Amazirh et al., 2024; Soltani, 2025). Additionally, the huge but limited opportunity to share data among nations as well as data collection and processing costs (Seyoum et al., 2019) further contribute to the hindrances faced.

The gravity recovery and climate experiment (GRACE) project was initiated in March 2002 (Rodell and Famiglietti, 2001) and followed by its sister GRACE-Follow-On (GRACE-FO) in 2018. GRACE is the first global-scale satellite project of its kind that paved the way for monitoring water storage variations on the Earth. The gravity signals gathered by the GRACE satellites go through multi-step processing to yield monthly TWS data (Khorrami and Gunduz, 2021a, 2021b; Ali et al., 2021a, 2021b; Ali et al., 2024b; Khorrami et al., 2023a). Although the inherent spatial resolution of TWS estimates is $3^\circ \times 3^\circ$, they are represented at finer grid sizes ranging from $1^\circ \times 1^\circ$ to $0.25^\circ \times 0.25^\circ$ (Khorrami and Gündüz, 2023; Ait Dhmane et al., 2024).

Notwithstanding their successful applications over large scales, the local-scale applications of the GRACE TWS are shackled on the grounds of their coarse spatial resolution (Soltani et al., 2020, 2021; Fatolazadeh et al., 2022; Rafik et al., 2023). Therefore, downscaling is a mandatory practice when dealing with local-scale GRACE-based analysis. Machine learning (ML) models are frequently being used for downscaling satellite data, particularly GRACE estimates. These models depend on statistical relationships between large- and local-scale hydro-meteorological variables (Wilby et al., 2004). The hydrological modeling enables the simulation of high-resolution parameters, thereby facilitating the integration of high-resolution modeling outputs. These outputs can be employed subsequently to enhance the spatial resolution of response variables, such as GRACE TWS. Statistical downscaling techniques are aimed at providing finer details of a parameter, which best depicts its local-scale variations. It is, therefore, essential to compare results obtained from various hydrological models to enhance our comprehension of which model offers the most accurate assessment for TWS variations at a local scale.

To date, many researchers have done GRACE satellite data downscaling using different ML statistical techniques. Notwithstanding the variations in the performance of the used techniques, they all

have one thing in common, namely the application of the global and open-access hydrological modeling, mainly from Global Land Data Assimilation System (GLDAS), Famine Early Warning Systems Network Land Data Assimilation System (FLDAS), and WaterGAP (Long et al., 2016; Rahaman et al., 2019; Chen et al., 2019; Ali et al., 2021a; Khorrami et al., 2021, 2023b; Soltani et al., 2021, 2024; Yin et al., 2022a, 2022b; Khorrami, 2023; Tariq et al., 2023; Kim et al., 2024; Gou & Soja, 2024). Notwithstanding their widespread applications, these large-scale models use several parameters with specific parameterizations but introduce uncertainty due to simplifications and assumptions about land surface processes (Fisher and Koven, 2020) without considering the local-scale hydroclimatic dynamics. Consequently, the simulations conducted by researchers could potentially introduce larger uncertainties, as indicated by Jin et al. (2010), thereby contributing to the overall uncertainty of the downscaled results.

The ParFlow hydrological model represents a grid-based parallel integrated approach for hydrologic modeling, enabling the simultaneous simulation of flow above and beneath the Earth in a 3D framework (Maxwell et al., 2009; Soltani et al., 2022b). This model can be used for a variety of regional water problems over large and small basins. It does consider surface processes such as evaporation. Consequently, to produce more realistic outputs, ParFlow is often coupled with a land surface model, particularly the common land model (CLM) (Sulis et al., 2017). The coupled ParFlow-CLM (PFC) model operates at fine spatial resolutions, considering variations in topography, vegetation effects, and the impacts of the variations in land use and climate change (Soltani et al., 2022a). The model assesses water availability, ecosystem health, and hydrological processes, supporting water resources management strategies and enabling the evaluation of flood risk and water scarcity. With its comprehensive capabilities, the PFC serves as a valuable tool for studying hydrological systems and making informed decisions in various domains. In contrast to other hydrological models, the PFC model provides a more comprehensive and intricate account of the various components involved in the land surface energy mass balance (Koch et al., 2016). Consequently, this enhanced level of detail facilitates more accurate hydrological simulations (e.g., Soltani et al., 2022a).

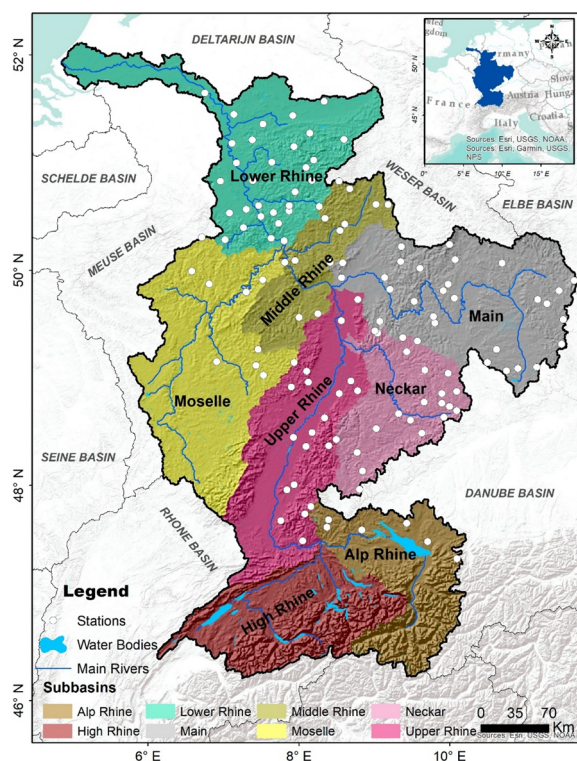


Fig. 1. Location of the Rhine Basin in Central Europe.

We postulate that employing a fully-coupled hydrological modeling approach for GRACE TWS downscaling could yield more accurate outcomes than using global models (such as FLDAS). The Random Forest (RF) ML model is very promising method of downscaling GRACE data, owing to its capacity to efficiently manage multiple input variables, achieve high accuracy, and effectively identify the weights of each variable (Chen et al., 2019; Rahaman et al., 2019; Mohtaram et al., 2024, 2025). In this premise and as a novel model-based downscaling approach, the PFC outputs are integrated into the RF model to derive high-resolution TWS values (0.1°) to better characterize water storage dynamics. The RF model is trained separately with outputs of the PFC and FLDAS models to downscale GRACE TWS. The study hypothesis is tested by the validity of the results against the in-situ observations.

THE STUDY AREA: GEOGRAPHIC AND HYDROCLIMATIC SETTINGS

The Rhine Basin in Central Europe covers a vast area of $163,500\text{km}^2$. It extends across nine

countries, namely Italy, Austria, Liechtenstein, Switzerland, France, Germany, Luxemburg, Belgium, and the Netherlands. Most of the basin, approximately two-thirds, lies within Germany (Fig. 1). The Rhine River, stretching approximately 1,200km in length, is the longest in Western Europe. Its source can be traced back to the lofty Alpine mountains in Switzerland, from where it meanders through numerous major urban centers and industrial areas before finally emptying into the North Sea in the Netherlands. The Rhine, along with its primary tributaries, holds significant economic advantages and cultural significance for the estimated 60 million inhabitants of Europe (Ullrich et al., 2021).

The temperate climate of the basin is characterized by an average annual temperature and precipitation of 8.3°C and 945mm, respectively. Both precipitation and temperature can show considerable variations according to altitude and local topography (Uehlinger et al., 2009). Precipitation in the basin can reach above 2,000mm in the mountainous areas (Ionita, 2017). The surface topography of the mountainous basin reaches up to 2,500m above sea level (asl). Thus, snow constitutes a significant proportion of total precipitation (37%) in this part of the basin, particularly in winter (Soltani et al., 2022a).

Data and Methodology

GRACE Observations

The data processing facilities for the GRACE project, such as the Center for Space Research at the University of Texas (CSR), the German Research Center for Geosciences (GFZ), and the Jet Propulsion Laboratory (JPL), are responsible for analyzing gravity signals and providing TWS estimates (Khorrami and Gunduz, 2021a). The Mascon solution approach is a technique used to process GRACE observations. It does not apply to the same extent of signal processing as spherical harmonics (SH) solutions. Instead, it utilizes predefined mascon blocks or grid locations for the estimation of mass variations. GRACE mascon solutions provide a more accurate, localized, and noise-free representation of Earth's mass variations compared to traditional SH solutions. This approach proves to be versatile, as it can be applied to various fields including hydrology, oceanography, and the cryosphere. Notably, it eliminates the need for any

postprocessing or filtering procedures as well as the application of empirical scaling factors (Save et al., 2016). Three different sets of GRACE mascon products from CSR, JPL, and Goddard Space Flight Center (GSFC) were utilized in this research. The initial GRACE data were obtained from <https://grace.jpl.nasa.gov/data/get-data/> for JPL and GSFC datasets and from https://www2.csr.utexas.edu/grace/RL06_mascons.html for the CSR dataset.

FLDAS Model

The FLDAS incorporates data obtained from field observations and remote sensing to create a comprehensive open-access global model that estimates a range of hydrometeorological parameters (McNally et al., 2017). The FLDAS simulates parameters using the variable infiltration capacity (VIC) and the Noah models, with resolutions of 0.01 and 0.25 degrees, respectively (McNally et al., 2017). The FLDAS–Noah model was utilized in this study to extract hydrometeorological parameters, including snow water storage (SWE), soil moisture storage (SMS), precipitation (P), temperature (T), runoff (R), and evapotranspiration (ET). These parameters were utilized as training inputs for the ML algorithm to estimate higher-resolution TWS. The FLDAS data were obtained from https://disc.gsfc.nasa.gov/datasets/FLDAS_NOAH01_C_GL_M_001/summary?keywords=FLDAS.

Reconstruction of GRACE Data Gaps

The GRACE mission does not offer a seamless dataset of global TWS. There are two kinds of gaps: individual gaps (mission gaps) and intermittent gaps (intermission gaps). The latter is the result of delay between the GRACE-FO and GRACE missions. In order to address the data gaps in the GRACE and GRACE-FO estimates, various ML techniques have been employed successfully to reconstruct the missing data (Mukherjee and Ramachandran, 2018; Zhang et al., 2021). Nonetheless, the predominant focus of these techniques on climatic variables raises concerns regarding their efficacy, as they may not accurately capture the fluctuations in GRACE TWS, which are influenced not only by climatic factors but also by human activities (Jing et al., 2020).

In this study, 15 (2003–2017) years of analysis were associated with 24 missing months, which were

reconstructed using the seasonal trend decomposition using loess (STL) technique (Khorrami et al., 2023c; Ali et al., 2024a). As a straightforward and potent filtering technique, the STL technique has been well-documented for breaking down time series datasets due to its simplicity and efficiency (Cleveland et al., 1990). The STL-based method presents a straightforward technique for addressing gaps in global TWS values. By decomposing the TWS time series into its various components, it is suggested that reconstructed TWS values may provide a more accurate representation and characterization of actual GRACE-observed TWSA features, incorporating both natural and anthropogenic effects (Ali et al., 2024a). The GRACE gaps were reconstructed using the seasonal and long-term characteristics of the TWS by applying the revised STL method. The STL initially breaks down the time series data into its constituent parts, thus:

$$\text{TWS}_t = \text{Trend}_t + \text{Seasonal}_t + \text{Residual}_t \quad (1)$$

Subsequently, it fills in the missing data by incorporating the mean seasonal and residual values, in addition to the trend component specific to the absent month, thus:

$$\text{TWS}_t = y (\text{Trend}_t) + \overline{\text{Seasonal}_t + \text{Residual}_t} \quad (2)$$

where $\text{Trend}_t + \text{Seasonal}_t + \text{Residual}_t$ denotes the trend, seasonal, and residual of TWS, respectively, at time t (Cleveland et al., 1990).

ParFlow –CLM Coupling

Model Description The PFC is an all-encompassing hydrological model that integrates the advantages of both the ParFlow model and CLM. By doing so, it can effectively simulate intricate interactions between land surface and subsurface hydrology. This specialized model is particularly tailored to precisely simulate movements of water and energy across vast geographical areas at high spatial resolutions (Sulis et al., 2017).

The PFC model incorporates two key components. The first is the ParFlow model, which solves the Richards equation governing water flow through 3D variably saturated porous media (Jones and Woodward, 2001; Maxwell et al., 2016). This equation accounts for various factors like soil properties, topography, and vegetation impacts to simulate subsurface water movement. ParFlow employs a fi-

nite difference approach and parallel computing to efficiently handle the complex computations involved (Kollet and Maxwell, 2006). On the other hand, CLM (v. 3.5) (Oleson et al., 2008) focuses on representing land surface processes. It consists of modules dedicated to surface energy balance, vegetation dynamics, biogeochemistry, and snow accumulation and melt. These modules interact with the ParFlow subsurface component through flux exchanges, enabling processes like water infiltration from the surface to the subsurface, evapotranspiration from vegetation, and heat transfer between the land surface and subsurface to be effectively simulated and integrated into the model (Soltani, 2022).

ParFlow contributes detailed subsurface variables such as groundwater levels, soil moisture profiles, and subsurface flow rates. These variables provide CLM with a more accurate representation of the below-ground hydrological dynamics, allowing for improved estimation of water availability for vegetation and evapotranspiration processes. In return, CLM supplies ParFlow with surface variables, including precipitation, temperature, incoming radiation, and vegetation characteristics (Kollet and Maxwell, 2006). These surface variables influence ParFlow's simulations by affecting infiltration rates, soil moisture recharge, and overall subsurface water movement. The exchange of these variables between ParFlow and CLM forms a dynamic feedback loop, enabling a more comprehensive understanding of how subsurface and surface processes interact and shape the overall behavior of the terrestrial ecosystem (Soltani, 2022). The ParFlow model transfers the updated relative saturation (S_w) and pressure (ψ) values for the top 10 soil layers to the CLM. In response, CLM sends the depth-differentiated source and sink terms for soil moisture, including the top soil evapotranspiration (q_e) and soil moisture flux (q_{rain}) for the top 10 soil layers back to ParFlow. This integrated approach ultimately enhances our ability to study and predict complex interactions within the coupled hydrological-ecological system. The model visualization in Figure 2 showcases its structure and configuration.

Atmospheric Forcing Input Data The land surface consists of static parameters such as topography, land use/cover (LULC), soil properties, and the canopy's physiological factors (Table 1). The researchers employed the Global Multi-resolution Terrain Elevation Data (GMTED) 2010, with a resolution of 0.01° , to generate the digital elevation model (DEM). For land use classification, the

MODIS data (Friedl et al., 2002) were employed and transformed into plant functional types (PFT). Soil properties were integrated by acquiring data on the proportion of clay and soil from the FAO/UNESCO global data repository (Batjes, 1997). The Soil Grids 0.0025° dataset, which has been aggregated to a resolution of 0.01° , was utilized to examine the hydraulic properties of soil, including saturated hydraulic conductivity and Van-Genuchten parameters. European pedotransfer functions (EU-PTFs) were employed to derive these hydraulic properties. A suggested association between land cover type and Manning's coefficient was applied by researchers based on the study by Soltani et al. (2022a).

To acquire meteorological information, scientists made use of data from the German Weather Service. These data encompass various parameters such as wind speed, specific humidity, barometric pressure, longwave radiations, downward shortwave, and precipitation, as well as the air temperature close to the Earth's surface. This study applied the PFC model utilizing daily atmospheric forcing data with resolution of $0.1^\circ \times 0.1^\circ$ from the COSMO-REA12 databank. The COSMO-REA12 dataset includes the CORDEX EUR-11 domain and encompasses data from the period spanning 2003 to 2017. Notably, the COSMO-REA12 dataset is a reanalysis data with high resolution obtained from the Hans-Ertel Center for Weather Research, making it a valuable resource for this research.

Simulation Setup A 15-year simulation was conducted utilizing the PFC model to assess the model's effectiveness in representing hydrologic states and fluxes across the Rhine Basin. The study focused on the Rhine Basin, and the model considered different thicknesses over its model layers to achieve a total thickness of 50m. The soil layers in the model increase in thickness with depth. The soil grids offer information on hydraulic properties, specifically the saturated hydraulic conductivity and Van-Genuchten parameters, for up to 2 m of soil depth. For deeper layers, the hydraulic characteristics were assumed to be the same as those at 2m depth below the surface. The ParFlow enables the user to define values for the permeability tensor. For this study, the permeability was considered to be heterogeneous and equally distributed across the three dimensions (x, y, and z). The permeability values were defined across the entire domain and were assumed to be isotropic (Soltani et al., 2022a). To achieve dynamic equilibrium, the hydrological

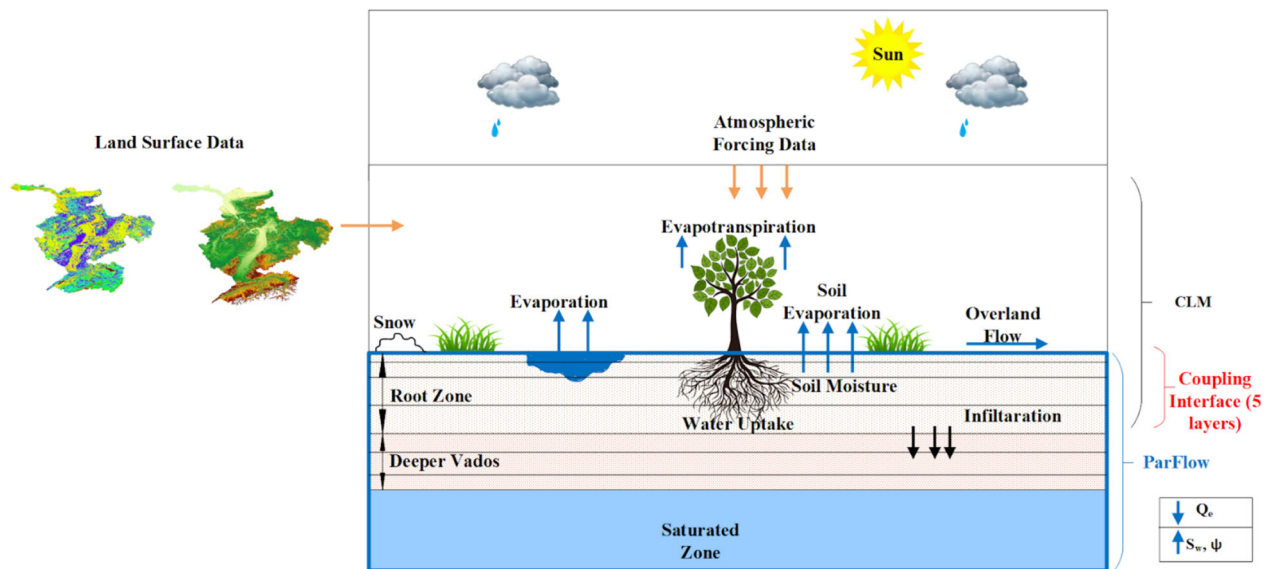


Fig. 2. PFC model. The coupling of hydrologic components is visually emphasized in the diagram, showcasing how the ParFlow model and CLM work in tandem, effectively exchanging information and data to provide an integrated simulation of the hydrological processes.

Table 1. Characteristics of data used for PFC modeling

Dataset	Source	Resolution	Reference
Atmospheric forcing	COSMO-REA12	0.1°	ftp://ftp-cdc.dwd.de/pub/REA/
Plant functional type	MODIS	0.005°	https://lpdaac.usgs.gov/products/mcd12q1v006
Soil texture	FAO/UNESCO Digital Soil Map of the World	0.0025°	Batjes (1997)
Saturated hydraulic Conductivity and Van-Genuchten's Parameter	European Soil Data Centre (ESDAC)	0.01°	https://esdac.jrc.ec.europa.eu/content/3d-soil-hydraulic-database-europe-1-km-and-250-m-resolution
DEM	GMTED2010	0.01°	https://earthexplorer.usgs.gov/
Manning's coefficient	Relationship between land cover type and Manning's coefficient	0.005°	Soltani et al. (2022a)

parameters of the PFC mode were continuously simulated through the designated modeling configuration. The simulation, commonly referred to as a spin-up run, was conducted to achieve a stable and rational distribution of the initial state variables. To accomplish this, the year 2003 was simulated 10 times, resulting in a spin-up period of 10 years. This approach aligns with previous studies of Soltani (2022). The PFC model was ran continuously following the spin-up until the total water storage change was below 2% in comparison to the preceding years. The resulting initial conditions of steady-state were subsequently employed in model simulations spanning from 2003 to 2017.

Generalized Three-Cornered Hat Method

The Generalized Three-Cornered Hat (GTCH) algorithm (Tavella and Premoli, 1994) has the capability to handle data with correlations when appropriately constrained (Tavella and Premoli, 1994). The assumption of this technique is that observations consist of a common signal but with uncorrelated noises (Tavella and Premoli, 1994). The GTCH algorithm was applied to calculate the associated uncertainties of GRACE mascon products relative to each other to come up with the least contaminated GRACE observations over the study area. The GTCH is formulated as follows.

The time series of the GRACE dataset is expressed as:

$$\text{GRACE}_i = \text{GRACE}_t + \varepsilon_i, i = 1, 2, 3, s, N \quad (3)$$

where N denotes the number of GRACE mascon products ($N=3$ for this study), GRACE_i is the time series of the i th GRACE product, GRACE_t signifies the original value of GRACE, and ε_i is the zero-mean white noise of the i th GRACE product. The GRACE_t value is missing; therefore, one of the GRACE products was chosen randomly as the reference product, against which the time series differences of the other GRACE products were calculated (Koot et al., 2006), thus:

$$Y_i = \text{GRACE}_i - \text{GRACE}_r = \varepsilon_i - \varepsilon_r, i = 1, 2, 3, s, N - 1 \quad (4)$$

The reference product's time series (CSR mascon for this research) is denoted as GRACE_r . The uncertainty linked to each GRACE product is theoretically independent of the reference product selection, as the GTCH method is not sensitive to it (Koot et al., 2006; Duan et al., 2024). For in-depth explanation of this approach, see Koot et al. (2006) and Duan et al. (2024).

Machine Learning Downscaling of GRACE TWS

RF is a ML technique that utilizes ensemble-based classification and regression trees (CART) for predictive analysis. It is composed of a set of CARTs whose strength determines the precision of RF-based predictions (Habibi et al., 2023). The RF employs a stochastic approach to construct a regression tree by utilizing a collection of random homogeneous subsets of predictors. It subsequently applies the average of the results obtained from every decision tree (Rahaman et al., 2019). The RF model can handle a multitude of input data, is highly accurate, and can determine the importance of variables (Chen et al., 2019; Rahaman et al., 2019). Thus, it has been used pervasively in hydrology and remote sensing.

The downscaling process is as follows: Initially, all input parameters are aggregated to the spatial resolution of the GRACE-CSR mascon, specifically $0.25^\circ \times 0.25^\circ$. The subsequent analysis investigates the statistical correlations between TWS and various hydro-meteorological factors, including P, T, SMS, ET, R, and SWE, utilizing data from both the

FLDAS and PFC models at the same $0.25^\circ \times 0.25^\circ$ resolution. This is achieved through the construction of a RF model designed to predict TWS. Following this, the residuals are determined by subtracting model-derived TWS from TWS obtained from GRACE. The developed model is then applied to the hydrometeorological parameters at a higher resolution of $0.1^\circ \times 0.1^\circ$, which results in an estimated TWS at that resolution. A residual correction is subsequently performed at $0.1^\circ \times 0.1^\circ$ by adding the calculated and interpolated ($0.1^\circ \times 0.1^\circ$) residuals to the estimated TWS, thus producing the downscaled TWS ($0.1^\circ \times 0.1^\circ$) (Fig. 3).

The residual correction methodology is structured into three sequential steps: (1) re-aggregation of fine-scale predictors ($0.1^\circ \times 0.1^\circ$) to the original TWS resolution ($0.25^\circ \times 0.25^\circ$); (2) determination of TWS residuals by evaluating the differences between the newly created coarse-scale predictor datasets and the GRACE TWS data; and (3) resampling of the residuals through bilinear interpolation, followed by their addition to the fine-resolution predicted TWS, which produces the final downscaled TWS values ($0.1^\circ \times 0.1^\circ$). This residual correction procedure is crucial for ensuring that the downscaled TWS corresponds accurately to the GRACE TWS data and mitigates any potential prediction bias due to omitted parameters.

Validation

To evaluate the precision of the results, three widely utilized accuracy metrics such as the Nash-Sutcliffe model efficiency coefficient (NSE), root mean square error (RMSE), and the correlation coefficient (CC), were applied. The downscaled TWS values were validated against high-resolution water storage anomalies (HWSA) (Zhang et al., 2024) and the field observations of P. The P data were obtained from 128 rain gauge stations spread over the basin. The Deutscher Wetterdienst (DWD) company in Germany administers these stations. The rain gauge stations were almost uniformly distributed over the majority of the basins, though poorly distributed over the Moselle and Alp Rhine basins. There is no station accessible for the High Rhine basin. These poor distribution and data scarcity issues stem from the fact that these basins fall beyond Germany's boundaries and, therefore, are not administrated by the DWD. The data can be

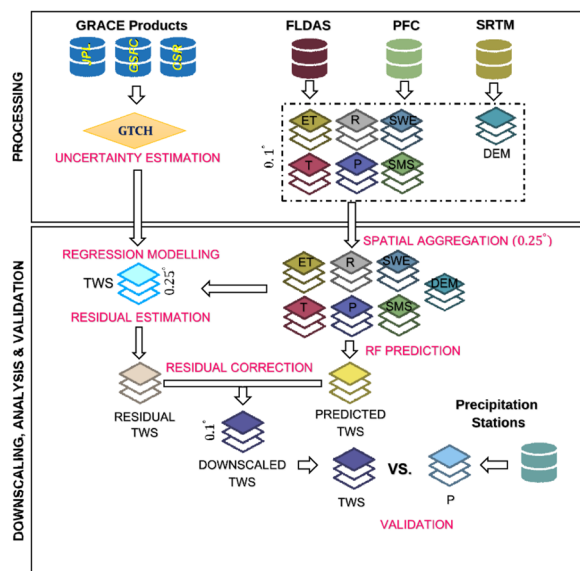


Fig. 3. Schematic illustration of the downscaling analysis workflow.

accessed on https://opendata.dwd.de/climate_environment/CDC/observations_germany/climate.

RESULTS

Uncertainty Estimation by GTCH Algorithm

The GTCH algorithm measures unsystematic errors through the use of at least three separate time series of a single parameter (Chen et al., 2021). The GTCH algorithm estimated the uncertainties of the three GRACE mascon datasets from 2003 to 2017. Figure 4 depicts the grid-based uncertainties associated with the CSR, JPL, and GSFC mascon products over the Rhine Basin. From basin-wise perspective, the CSR product typically has the smallest uncertainties, while the GSFC product tends to have the largest uncertainties. Overall, it can be stated that the low estimation errors in the CSR product are due to its efficient and user-friendly data processing algorithm through which more spatial details and higher apparent resolution estimates are offered (Jing et al., 2019).

The uncertainties of the three GRACE mascon products are also depicted as boxplots (Fig. 5). The JPL exhibited uncertainties ranging 1.27–4.30mm while the GSFC showed uncertainties ranging 1.64–4.70mm. In addition, the uncertainties in the CSR ranged 0.45–3.50mm. The medians (maxima) of the

JPL, GSFC, and CSR products were 2.86mm (3.66mm), 3.22mm (4.03mm), and 2.0mm (2.86mm), respectively. Based on these results, we selected the GRACE CSR mascon product for further analysis.

Downscaling Performance

The TWS values received from the CSR data were downscaled based on the two downscaling scenarios. In the first stage, the FLDAS model outputs were integrated into the RF model, and in the second scenario, the output parameters obtained by the PFC-model simulation were applied in the RF model. For a better illustration of the modeling results, the input variables received from the FLDAS and PFC models are shown in supplementary Figure SM1. To appraise the efficacy of the downscaling approaches, the GRACE and downscaled TWS values were compared (Fig. 6). The accuracy of the downscaling results was demonstrated through three statistical metrics: R, RMSE, and NSE. The findings suggest that the FLDAS-based approach simulates the TWS with a coefficient of correlation (CC) of 0.80, NSE value of 0.64, and RMSE of 38.10mm. The PFC-based approach, on the other hand, shows a far better performance with a coefficient of determination of 0.98, NSE value of 0.96, and RMSE of 7.05mm.

The spatial coherence of the TWS before and after downscaling was evaluated as another means of examining the downscaling performance. To this end, the distribution of the mean annual TWS from the GRACE-CSR and the downscaled TWS time series were plotted over the study area (Fig. 7). It suggests that the PFC-based downscaled TWS values demonstrate a pattern resembling the spatial dispersion of the GRACE-CSR TWS over the basin. On the other hand, the distribution of the FLDAS-based downscaled TWS is divergent from the GRACE-CSR TWS values indicating that the proposed PFC model-based downscaling approach outperforms the FLDAS-based in simulating the local-scale variations of TWS.

The downscaling precision was further investigated based on the multi-year (2003–2017) trend analysis results (Table 2). The trends of the GRACE-CSR TWS were used as reference to check the precision of the trends estimated based on the downscaled TWS. Based on the results, the PFC-based downscaled TWS gave better estimates of long-term trend values in comparison with the

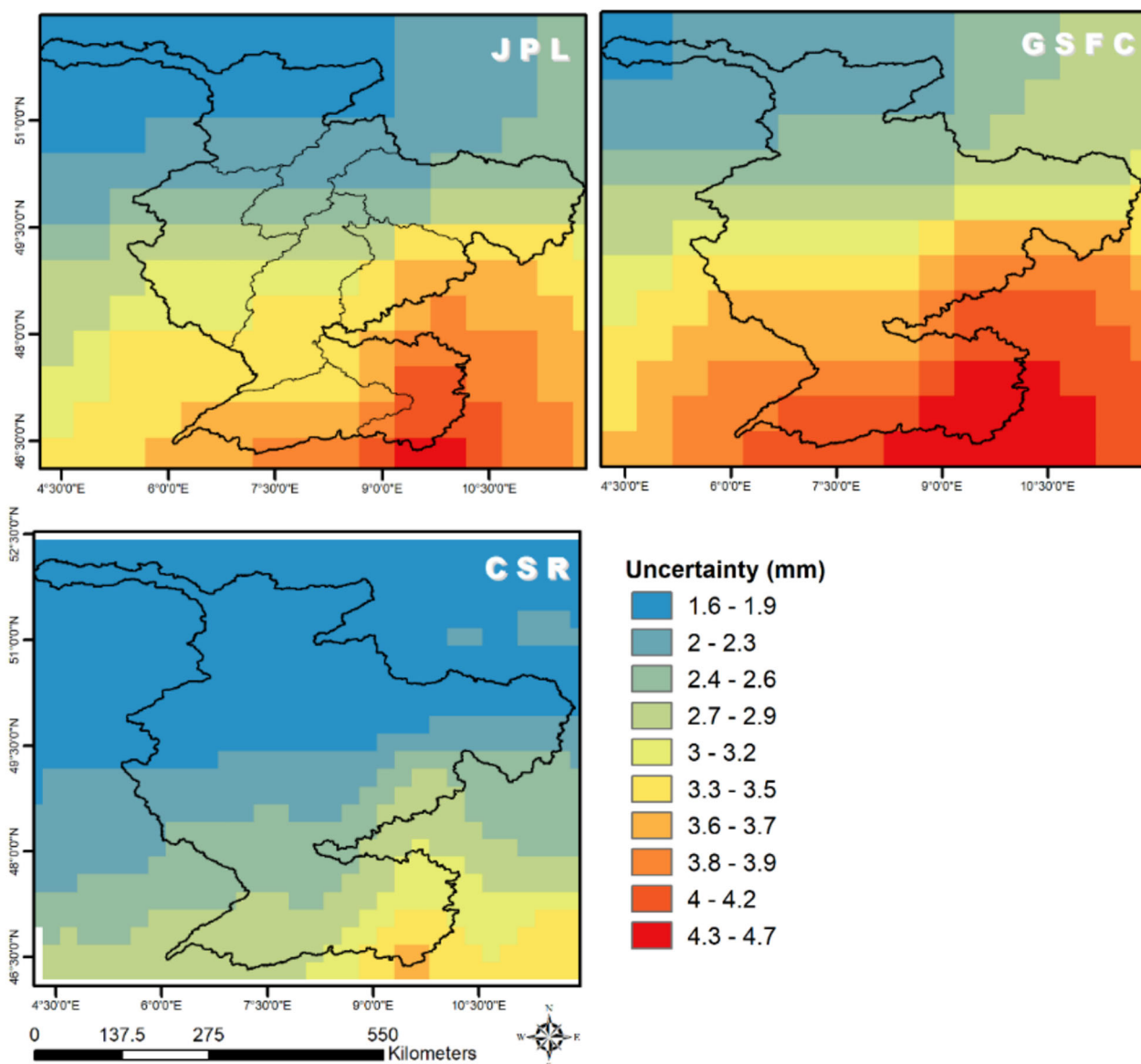


Fig. 4. Uncertainties in GRACE mascon products (JPL, GSFC, and CSR) over the Rhine Basin (2003–2017).

FLDAS-based TWS time series, suggesting better performance by the PFC-model approach (Table 2). The FLDAS-downscaling approach demonstrated weaker performance in capturing the variations of TWS, especially over the Lower Rhine, Middle Rhine, and Main basins, for which there is a considerable discrepancy in the estimated trend values. While the original TWS in the Lower Rhine, Middle Rhine, and Main basins showed diminishing trends of -1.73mm , -2.40mm , and -2.48mm , the FLDAS-based downscaled trends were much higher, namely

-2.70mm , -2.88mm , and -2.92mm of water loss, respectively.

Validation Against Precipitation Data

The local-scale hydroclimatology of the basin is characterized by field-based precipitation data. To validate the downscaling results, monthly data from rain gauges were used to evaluate their associations with downscaled TWS values. A station-wise approach was applied in the validation process, and the

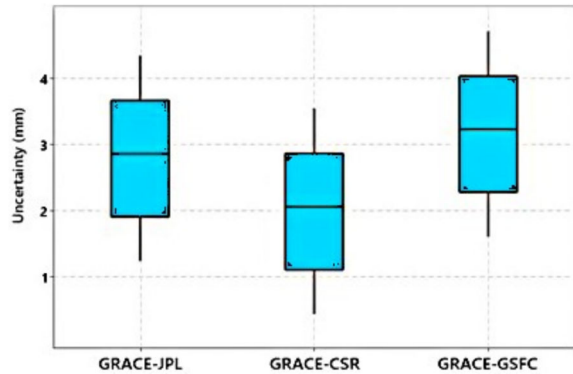


Fig. 5. Boxplots of the uncertainties measured in JPL, CSR, and GSFC products.

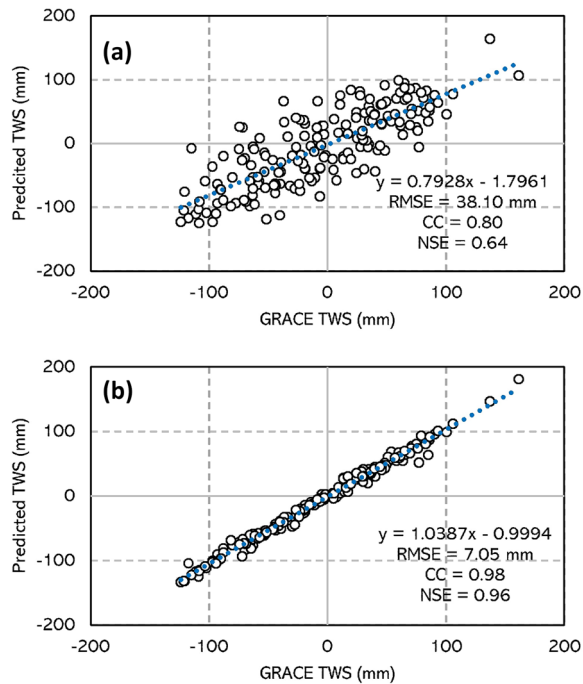


Fig. 6. Comparison of GRACE CSR TWS (x axes) with predicted TWS (y axes) obtained from (a) FLDAS modeling and (b) PFC modeling.

average number of stations was calculated for each basin. Because no station is accessible for the High Rhine basin, the validation analysis for this basin is lacking. Figure 8 portrays the temporal associations between the downscaled TWS and averaged precipitation gauges for both hydrological models. The findings indicate that the signals produced by the fully-coupled hydrological model exhibited slightly superior performance compared to FLDAS model in terms of accurately representing water storage

fluctuations at local scales, as evidenced by their stronger associations with the field-based data. Under the PFC model-based downscaling scenario over the study basins, the RF prediction produced higher CC values ranging 0.47–0.60 (Fig. 8b) whereas the FLDAS model-based downscaling produced lower CC ranging 0.37–0.50 (Fig. 8a). This findings align with the precision evaluation of the ML algorithms (Fig. 6).

Validation Against HWSA Dataset

The results were further validated against the HWSA v1.0 data generated by Zhang et al (2024) based on the integrated use of ML downscaling framework and physically constrained sliding window technique. The data cover the whole globe and offer TWS values at spatial resolution of 1–10 km, which is accessible at 国家青藏高原科学数据中心 (<http://tpdc.ac.cn/>). The temporal associations between the downscaled TWS and the HWSA data across the sub-basins of the study area are given in supplementary Figure SM2. The statistical results (Table 3) revealed that the basin-averaged TWS values from the PFC-based model had better correlations with the HWSA dataset than those from the FLDAS-based approach. The superiority of the PFC-based downscaling approach is demonstrated, in particular, by RMSEs, which showed lower differences from the benchmark dataset across all the sub-basins compared to the FLDAS-based downscaling approach.

Estimation of Water Storage Loss

To draw a clear picture of the water storage dynamics over the 15 years of the study, volumetric changes in TWS over each basin (Table 4) were estimated by factoring in the pixel count and the corresponding area of each basin. It was found that the Moselle, Upper Rhine, High Rhine, Alp Rhine, and Main basins had the most critical status regarding total water storage loss of 12.69km^3 , 12.67km^3 , 11.48km^3 , 10.68km^3 , and 10.27km^3 respectively, from 2003 to 2017. The results also revealed that the situation over the Neckar basins is relatively moderate, with total water loss of 7.30km^3 . The Lower Rhine and Middle Rhine basins with storage losses of 6.86km^3 and 4.30km^3 , respectively,

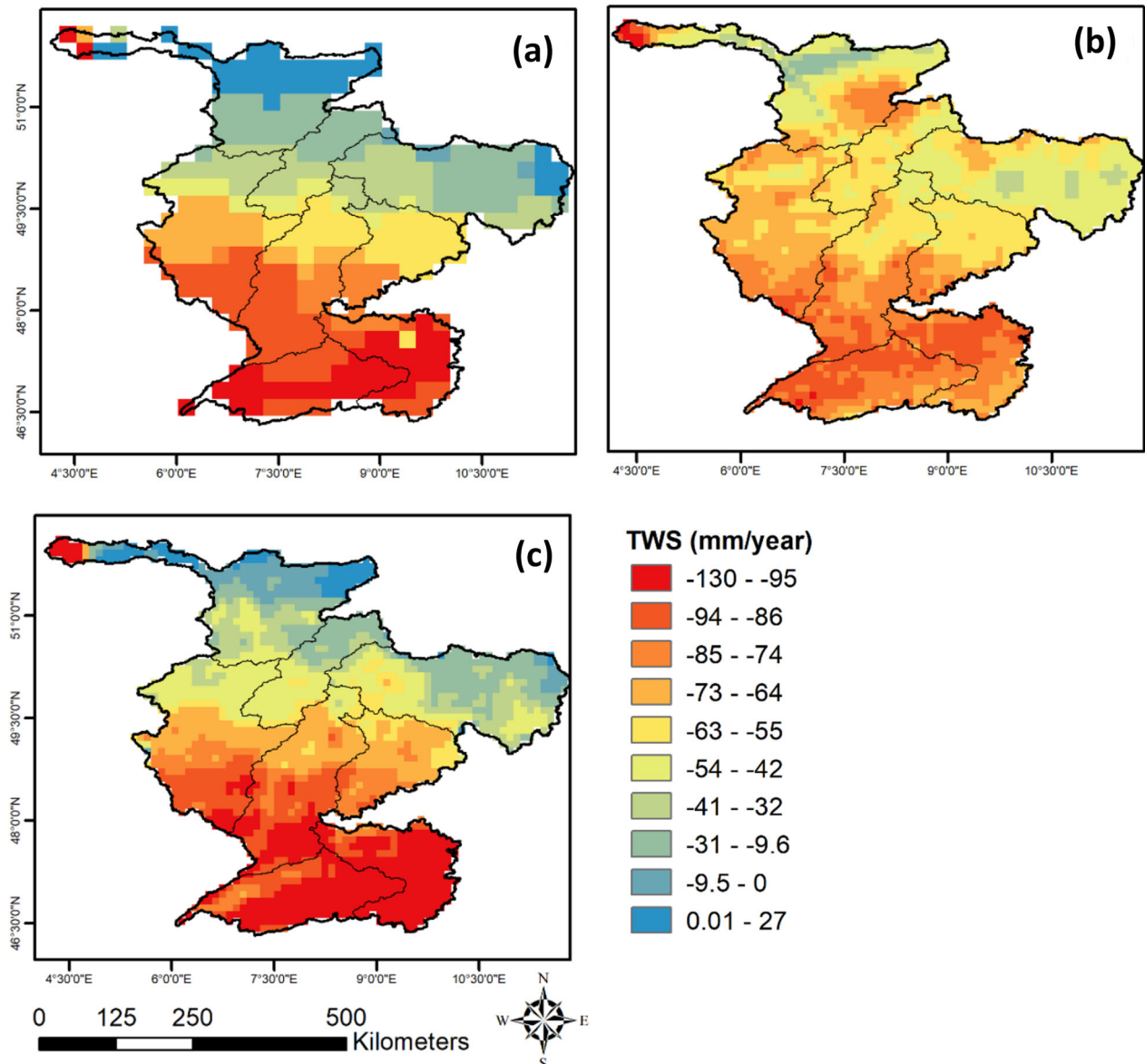


Fig. 7. Fluctuations of TWS (2003–2017) based on (a) GRACE-CSR, (b) FLDAS-based downscaling, and (c) PFC-based downscaling.

turned out to suffer the least from the water storage variations compared to the other basins (Table 4).

DISCUSSION

It is challenging to accurately determine uncertainties linked to GRACE estimates because no field-based data are available for validation. Therefore, actual uncertainties of values derived from mass changes of the Earth through this mission are still unknown (Chen et al., 2021). Despite the

possibility of validation by comparison with data like water storage changes from altimeter data or in situ measurements (e.g., Argus et al., 2020; Chen et al., 2021), as well as mass loads derived from GNSS data (Fu et al., 2015), it is important to acknowledge that each validation technique comes with its own set of constraints.

The GRACE mascon products were assessed for uncertainties using the GTCH algorithm. The results obtained indicated that the CSR mascon product had the least estimation error compared to the JPL and GSFC products. These findings align

perfectly with the researches of Sakumura et al., (2014), Ferreira et al., (2016), Chen et al. (2021), and Ferreira et al. (2023), who reported the smallest uncertainties for CSR products over the globe. The findings also indicate large uncertainties for JPL and GSFC compared to CSR, from which the GSFC turned out to be associated with the highest estimation errors. Ferreira et al. (2023) also reported large uncertainties for the JPL and GSFC mascon products on global and basin scales. The distributions of uncertainties in CSR, JPL, and GSFC products (Fig. 4) are relatively similar, with the lowest estimation errors over the north and the highest errors in the south of the basin.

To validate downscaled TWS over the basin, precipitation observations from rain gauges were applied as reference datasets. The comparisons were implemented on a temporal scale and based on a point-wise approach by using only pixel values extracted at the location of each rain gauge. Overall, the findings suggested better associations between precipitation and TWS over all the basins of the study area when integrating the PFC outputs into the RF model. The limited number of rain gauges shackled this analysis over some of the basins, which may have affected the results obtained. We suggest that using a denser rain gauge network would be beneficial in validating the TWS values against precipitation. It seems that even much better results are accessible in case of having a better comparison approach, such as grid-to-grid evaluation (Wolkeba and Mekonnen, 2024), which also enables spatial comparisons to draw more realistic analogies between the variations of TWS and precipitation. In this study, the point-wise nature of the precipitation data was ruled out when performing such a grid-wise comparison.

The analysis of the current study may also be affected by uncertainties induced by various sources of error. The original GRACE data are associated with inherent processing errors. The authors tried to get around this problem by applying GRACE mascon data, which seems to outperform the SH data (Aryal and Zhu, 2020). The authors further tried to select the best GRACE mascon data in terms of the associated uncertainties to reduce the possible impacts of errors on the analysis results by using the GTCH algorithm. Another error source is the gap-filling technique used to reconstruct the GRACE missing months. However, given its ease of application and good performance (Ali et al., 2024a), pervasive applications in hydrology, the GRACE missing values were reconstructed by applying the STL method. Uncertainties linked to hydrological models employed in generating high-resolution predictors for downscaling techniques might also affect the results. Using the ensemble mean of several hydrological model outputs is recommended to circumvent the uncertainty issue (Cao et al., 2015). Nevertheless, as a result of the limited availability of global hydrological models operating at a spatial resolution of $(0.1^\circ \times 0.1^\circ)$, the FLDAS was exclusively utilized in the analysis. Although the FLDAS model is a valuable global model, its performance is shackled by some technical issues. The precision of FLDAS outputs is significantly influenced by the quality of the input meteorological data, including parameters such as P and T. In areas where observational networks are limited, dependence on satellite or reanalysis data may lead to uncertainties. For instance, the FLDAS-global model utilizes CHIRPS precipitation data for latitudes between 50° S and 50° N, while employing GDAS or MERRA-2 precipitation inputs for regions outside these lati-

Table 2. Basis-wise trend of TWS (2003–2017)

Basin	TWS (mm/year)		
	GRACE-CSR	FLDAS-based downscaling	PFC-based downscaling
Lower Rhine	-1.73 ± 0.65	-2.70 ± 1.79	-1.79 ± 0.75
Moselle	-3.12 ± 1.90	-3.22 ± 2.80	-3.00 ± 1.99
Middle Rhine	-2.40 ± 1.43	-2.88 ± 3.70	-2.47 ± 1.67
Main	-2.48 ± 1.70	-2.92 ± 2.24	-2.49 ± 1.75
Upper Rhine	-3.68 ± 2.26	-3.53 ± 2.89	-3.61 ± 2.30
Neckar	-3.52 ± 2.50	-3.39 ± 2.83	-3.50 ± 2.54
High Rhine	-4.37 ± 2.95	-3.97 ± 3.50	-4.35 ± 3.00
Alp Rhine	-4.53 ± 3.03	-3.99 ± 3.91	-4.48 ± 3.21

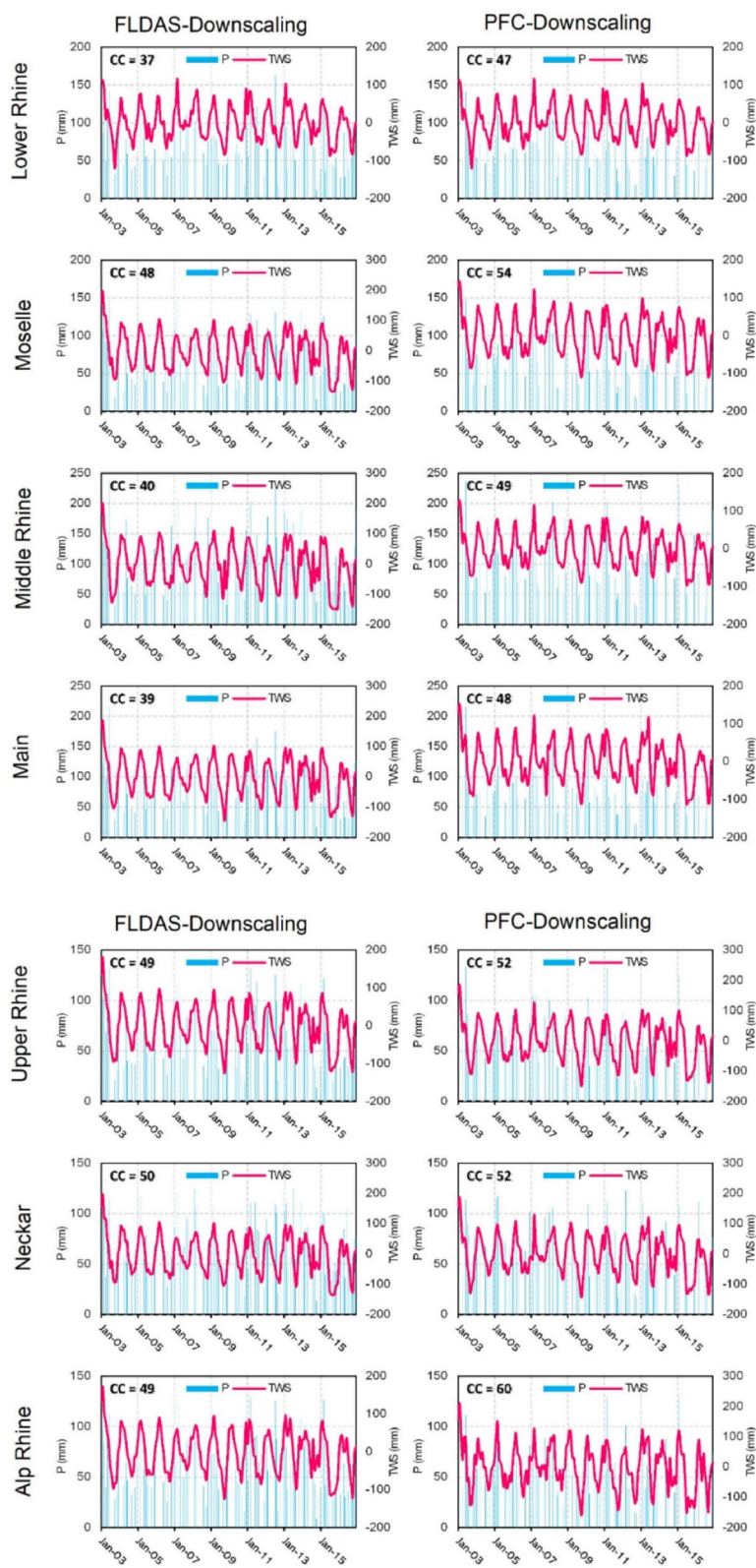


Fig. 8. Time series of the FLDAS-based downscaled TWS, PFC-based downscaled TWS, and rain gauge (P) (2003–2016).

tudes, potentially impacting the reliability of simulations in areas with insufficient data.

Furthermore, anthropogenic activities are excluded from the FLDAS simulation framework. This exclusion can create significant differences between simulated hydrological conditions and those observed in reality, especially in regions where human actions markedly modify water cycles. A study pointed out that contemporary land surface modeling systems, including FLDAS, do not integrate the effects of anthropogenic factors, potentially skewing the estimates of soil moisture, evapotranspiration, and streamflow (McNally et al, 2021). Model parameterization and calibration are other issues that may affect the accuracy of the simulations. The effectiveness of FLDAS is contingent upon the parameterization strategies integrated within its land surface models. When parameters are inaccurately defined or overly generalized, they can introduce

biases, particularly when the models are applied on a global scale that includes various climatic and ecological regions. As an illustration, there are ongoing efforts to upgrade to the Noah-MP land surface model, which entails recalibrating parameters associated with snow, glaciers, and groundwater to achieve greater precision (McNally et al, 2021). The authors believe it is crucial for related prospective studies to consider these limitations and influential factors such as data quality and representativeness. The primary emphasis of this research was on the datasets employed in statistical downscaling. In future investigations, more advanced methods like deep learning algorithms, in conjunction with an enhanced precipitation observation network, could be utilized to address the biases introduced by data and methodologies. Furthermore, the authors hold the notion that having an exhaustive analysis of the downscaling of the GRACE estimates under these

Table 3. Validation results of FLDAS-based TWS, PFC-based TWS, and HWSA (2003–2017)

		HWSA		
		CC	NSE	RMSE (mm)
Alp Rhine	FLDAS	0.94	0.87	0.09
	PFC	0.94	0.88	0.03
Lower Rhine	FLDAS	0.94	0.84	1.29
	PFC	0.95	0.92	0.52
Moselle	FLDAS	0.94	0.91	2.57
	PFC	0.94	0.91	2.08
Middle Rhine	FLDAS	0.95	0.91	1.87
	PFC	0.95	0.91	0.61
Main	FLDAS	0.92	0.87	1.94
	PFC	0.93	0.88	1.30
Upper Rhine	FLDAS	0.94	0.90	1.15
	PFC	0.94	0.90	0.87
Neckar	FLDAS	0.93	0.87	3.27
	PFC	0.93	0.87	2.92
High Rhine	FLDAS	0.93	0.87	0.48
	PFC	0.94	0.87	0.47

Table 4. Zonal statistics of volumetric TWS (2003–2017)

Watershed	Loss rate (mm/year)	0.1° Pixel Sum	Loss rate (km ³ /year)	Total Loss (km ³)
Lower Rhine	−1.79	254	−0.45	−6.86
Moselle	−3.00	282	−0.85	−12.69
Middle Rhine	−2.47	116	−0.29	−4.30
Main	−2.49	275	−0.68	−10.27
Upper Rhine	−3.61	234	−0.84	−12.67
Neckar	−3.50	139	−0.49	−7.30
High Rhine	−4.35	176	−0.77	−11.48
Alp Rhine	−4.48	159	−0.71	−10.68

two scenarios and incorporating different modeling outputs will cast more light on the feasibility of the model-based approach to get better results for local-scale water assessments.

CONCLUSIONS

The relatively coarse spatiotemporal resolution of GRACE observations significantly hinders their applicability in localized scenarios, particularly in the realm of hydrological assessments. Water resource managers and decision-makers prioritize the need to understand fluctuations in water storage at local scales. As a result, downscaling GRACE data is vital until upcoming missions can offer high-resolution estimates. The integration of additional data with enhanced spatial detail from diverse sources is essential for effective spatial downscaling initiatives, thereby improving the precision of estimates for the target variable. The data generated by hydrological models are ideally suited for incorporation into downscaling models. However, current research primarily utilizes outputs from global, publicly accessible hydrological models. This study, however, examined the viability of a surrogate scenario by leveraging auxiliary data obtained from fully-coupled physical hydrological modeling. Accordingly, high-resolution predictors in the PFC and FLDAS hydrological modeling were employed to downscale GRACE observations in the Rhine basin. By validating the results against the GRACE TWS and field-based precipitation observations, significant insights were gained regarding the hydrological model that most effectively represents local hydrological behavior and the methodology used. Due to its effective performance and broad range of applications, the RF ML algorithm was employed to downscale GRACE CSR data from a spatial resolution of $(0.25^\circ \times 0.25^\circ)$ to $(0.1^\circ \times 0.1^\circ)$, leveraging estimates from the FLDAS and PFC models.

To summarize, the study results revealed that downscaling GRACE TWS through the simulation outputs derived from the PFC model provides the most accurate representation of local hydrology, particularly in smaller basins. The downscaling method based on the PFC model, as proposed in this research, demonstrates both effectiveness and reliability within the Rhine basin, adhering to the necessary primary assumptions. This approach shows considerable potential for application in other river

basins worldwide. Moreover, given the performance of deep learning algorithms, integrating the outputs from the PFC model into these algorithms may lead to even more favorable results. The results indicated that this approach can be successfully employed to improve the accuracy and reliability of the down-scaled results in the test basin. Researchers worldwide may implement this methodology in their own fields of study. The proposed downscaling approach was developed using data derived from the PFC model, which can be implemented by scholars to replicate their specific parameters in their respective research areas.

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DATA AVAILABILITY

The data and codes supporting this study's findings are available upon a rational request from the corresponding author.

DECLARATIONS

Conflict of Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

SUPPLEMENTARY INFORMATION

Below is the link to the electronic supplementary material. Supplementary file1 (PDF 1767 KB)

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