

Article

The Extraction of Terrestrial Water Storage Anomaly from GRACE in the Region with Medium Scale and Adjacent Weak Signal Area: A Case for the Dnieper River Basin

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Abstract: The accuracy of estimating changes in terrestrial water storage (TWS) using Gravity Recovery and Climate Experiment (GRACE) level-2 products is limited by the leakage effect resulting from post-processing and the weak signal magnitude in adjacent areas. The TWS anomaly from 2003 to 2016 in the Dnieper River basin, with characteristics of medium scale and an adjacent weak TWS anomaly area, are estimated in this work. Two categories of leakage error repair approaches (including forward modeling, data-driven, single, and multiple scaling factor approaches) are employed. Root mean square error (RMSE) and Nash–Sutcliffe Efficiency (NSE) are used to evaluate the efficiency of approaches. The TWS anomaly inverted by the forward modeling approach (FM) is more accurate in terms of RMSE 3.04 and NSE 0.796. We compared single and multiple scaling approaches for the TWS anomaly and found that leakage signals mostly come from semi-annual terms. From the recovered results demonstrated in the spatial domain, the South of Dnieper River basin is more sensitive to the leakage effect because of it is adjacent to a weak hydrological signal region near the Black Sea. Further, comprehensive climate insights and physical mechanisms behind the TWS anomaly were confirmed. The temperate continental climate of this river basin is shown according to the variation in TWS anomaly in the spatial domain. Snowmelt plays a significant role in the TWS anomaly of the Dnieper River basin, following the precipitation record and the 14-year temperature spatial distribution for February. We compared single and multiple scaling approaches for the TWS anomaly and found that leakage signals mostly come from semi-annual terms.

Keywords: GRACE; terrestrial water storage (TWS) anomaly; leakage error recovery; Dnieper River basin; climate pattern



Citation: Zhang, T.; Bian, S.; Ji, B.; Li, W.; Zong, J.; Yuan, J. The Extraction of Terrestrial Water Storage Anomaly from GRACE in the Region with Medium Scale and Adjacent Weak Signal Area: A Case for the Dnieper River Basin. *Remote Sens.* **2024**, *16*, 2124. <https://doi.org/10.3390/rs16122124>

Academic Editors: Liming He and Gabriel Senay

Received: 13 April 2024

Revised: 19 May 2024

Accepted: 9 June 2024

Published: 12 June 2024



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1. Introduction

Terrestrial water storage (TWS), the summation of surface water, soil moisture, ground-water, ice, snow, and biosphere, is the critical component of the water cycle [1]. Reliable inversion of the TWS anomaly plays a key role in understanding the global or regional hydrological process and provides crucial information for water management. The in situ measurements of TWS limit the research on regional hydrological TWS anomaly. This is because current measurement methods and the characteristics of point-wise observation cannot obtain all of the TWS anomaly components. Along with rapid remote sensing development, particularly the implementation of the Gravity Recovery and Climate Experiment (GRACE) satellite mission, global or regional TWS research is possible. GRACE and its successor GRACE Follow-on (GRACE-FO) have provided precise observations of the global temporal gravity field for the first time, allowing access to detect the TWS anomaly directly.

In practice, the monthly gravity fields, sets of spherical harmonics coefficients (SHCs) truncated at a certain degree, are used to infer regional TWS anomaly. However, the SHCs provided by the GRACE RL-2 products should be filtered because of the inherent noise, including N-S “stripes” noise and short wavelength noise. The first filter, the Gaussian filter dedicated to solving short-wavelength noise, was devised by Wahr et al. [2]. It is an isotropic filter that only depends on the degree. Some non-isotropic filters have been proposed in the literature. Based on the Gaussian filter, Han et al. have developed a filter that reconstructs the averaging radii as a function of order, in which the averaging process depends on the degree and order [3]. Swenson and Wahr designed a filter to remove the stripes noise so that the correlated errors are fit by a polynomial with an empirical moving window [4]. Following the ideal of Swenson and Wahr, Chambers and Chen modified it more concisely. They left some portion of spherical harmonic coefficients unchanged, then fit the remnant even and odd coefficient pairs by the least squares and remove a polynomial of order 4 [5–7]. Duan et al. introduced two additional empirical parameters to the window width formula used by Swenson and Wahr [8]. This refined approach is based on the error pattern of the SH coefficients but complicated the determination of the unchanged portion and window width. Zhang et al. devised another non-isotropic filter called the fan filter, a 2-D double filter that simultaneously includes degree and order [9]. There are many prior covariance-dependent filters, such as the variance-dependent filter and empirical orthogonal function filter [10,11], but we did not list them all.

The noise that existed in the SHCs was suppressed by amounts of filters that attenuated the signal as well. Moreover, the regional average process for basin scale research also dampens the signal’s amplitude. The leakage error has generally been divided into two types. One type is the “leakage-in” error, caused by signals from adjacent areas leaking into the one of interest. The other type is the “leakage-out” error, which signals leakage opposite to the “leakage-in” error [12]. In this work, we recognized leakage error as the discrepancy between the recovered results followed by the methods described in Section 3 and the reference results derived from Mascon products.

Many techniques or strategies have been proposed to repair signal attenuation and leakage errors. Generally, leakage error repair approaches are divided into model-independent and model-dependent. Hydrological or meteorological models are usually adopted for model-dependent approaches to calculate the scaling factor. Landerer and Swenson simulate the relationship between filtered and unfiltered global gravity fields by the model GLDAS-NOAH and infer the scaling factor [13]. Pokhrel et al. employed the GRACE results repaired by the scaling factor approach and assessed the role of groundwater in the Amazon water cycle [14]. The hydrological model PCR-GLOBWB is used to generate the scaling factor for recovering the TWS anomaly of the Yangtze River basin [15]. As convenient, it has been widely applied in global or regional TWS anomaly research. At the same time, it is dependent on certain hydrological models possessing discrepant performance in different regions.

The other leakage error repair approach category is model-independent without auxiliary model data. Baur and Sneeuw applied a methodology of point-mass modeling to evaluate Greenland ice mass loss to avoid leakage effects arising from the filter process [16]. Chen et al. have analyzed the mechanism of leakage error from the SH truncation and spatial filtering detail and devised a method of constrained forward modeling to counteract that error [17]. Mu et al. proposed an approach of Tikhonov regularization with the L-curve method to reduce the leakage effect based on the correction equation established by Tang [18]. They successfully estimated the mass change rate in Greenland and Antarctica [19]. Vishwakarma et al. confirmed that signal leakage affects the amplitude and the phase exhibited in the time domain. They proposed a strategy to approach attenuation and phase shift called the data-driven method [20,21].

Many approaches have been proposed for precise inversion of TWS anomaly on a regional scale. However, most research concentrated on regions or river basins like the Amazon, Greenland, Indus, Antarctica, Yangtze River, Tibetan Plateau, Congo, Nile,

and so on [22–31]. Those regions are characteristic of larger areas ($>10^6$ km²) or stronger signals attributed to mass changes. Even though some works in the literature focus on the medium and small basins [32], such as Finland, the Liao River basin, and the Aral Sea basin [33–36], distinct mass changes or redistributions are also demonstrated in those regions. However, rarely has the focus been switched to the regions with medium-scale and weak adjacent areas.

The climatic conditions in the Dnieper River basin are complex due to the spatial heterogeneity of precipitation from northwest to southeast, which impacts the temperate continental climate [37]. The complex climate feature will be captured by inversed TWS anomaly from the GRACE temporal gravity field. The main aim of this study is to repair the leakage error caused by the GRACE data post-processing, particularly in a medium-scale region like the Dnieper River basin with an adjacent area weak signal. To that end, two categories of leakage error repair approaches were tested. Furthermore, we try to reveal the comprehensive climate significance behind the TWS anomaly in terms of spatial and time domains by the inversed GRACE results combined with hydrological and meteorological data.

2. Materials

2.1. Study Area

The Dnieper River basin, shown in Figure 1, is one of the largest river basins in Europe and covers an area of 511 thousand km² [38]. The river basin spans three countries, Russia, the Republic of Belarus, and Ukraine, and includes many sub-streams [39]. The Dnieper River is perennial, originating from the south of the Valdai Hills in Russia, flows through Russia, Belarus, and Ukraine, and finally empties into the Black Sea 30 km southwest of Kherson [37]. The Dnieper River has four main tributaries, and six reservoirs are built along the river [40].

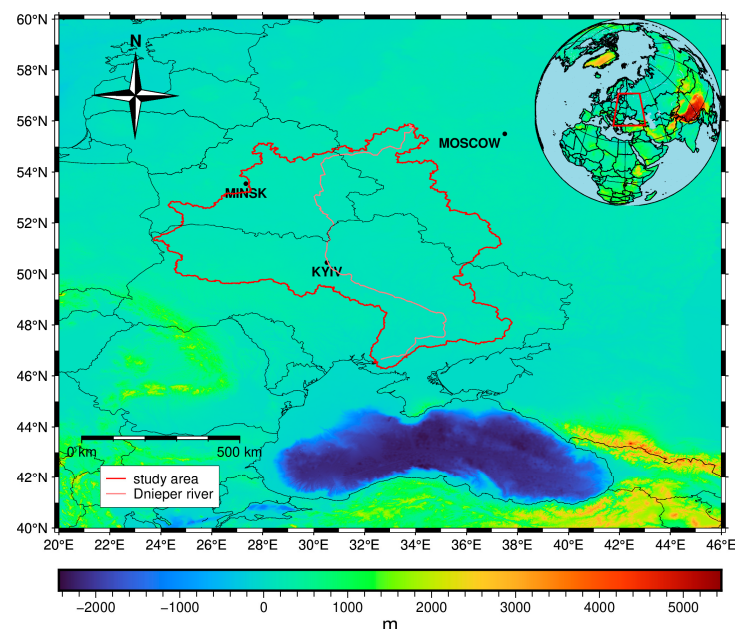


Figure 1. Topography of the Dnieper River basin. The area delineated by the red line is the study area, and the light red line represents the Dnieper River. The national capitals within or adjacent to the Dnieper River basin are shown with black dots: Kyiv, Minsk, and Moscow.

Conventionally, with Kyiv and Zaporizhzhia as the boundary, the Dnieper River has been decomposed into three parts (upstream, midstream, and downstream). The upstream is mainly located in a forest area with peat-podzolic soil. Additionally, this area has a well-developed river network, accounting for four-fifths of the annual flow of the whole basin,

with the most significant and longest tributaries, i.e., the Berezina River. The midstream and downstream are mainly covered by steppes with black soil. However, most of those regions have been reclaimed for agriculture.

The climate of the Dnieper River basin is warm and humid. From northwest to southeast, the continental climate is gradually prominent. The precipitation in this basin exhibits the properties of decreasing from north to south. Turning to the adjacent areas of the Dnieper River basin, the Black Sea is the distinctive region dominated by the Mediterranean climate. TWS anomaly of the Black Sea from GRACE is vulnerable to contamination from land hydrology due to the relatively weak fluctuation of mass change contrasted to adjacent land areas. Additionally, the Dnieper River basin is the leading region supplying crops for Europe, even globally. Considering climate and agriculture factors, the TWS anomaly estimated from GRACE for the Dnieper River basin is imperative.

2.2. Datasets

This work uses GRACE Level2 (Release 06) monthly gravity data sets combined with other climate and hydrological data sets to extract information about mass changes. Details of the data sets can be found in Table 1.

Table 1. List of the data sets (Data are all accessed on 12 April 2024).

Data Name	Data Version	Resolution	Period	Data Access
GRACE	CSR, R06L2	96 degrees and orders, monthly	2003–2016	https://isdc.gfz-potsdam.de/grace-isdc
Snow Water Equivalent	GLDAS Noah, version 2.1	1° by 1°, monthly	2003–2016	https://disc.gsfc.nasa.gov/
Soil Moisture	GLDAS Noah, version 2.1	1° by 1°, monthly	2003–2016	https://disc.gsfc.nasa.gov/
Total Water Storage	WGWM, Version 2.2d	0.5° by 0.5°, monthly	2003–2016	https://doi.pangaea.de/
Precipitation	GPCC, Full Monthly Version 2020	0.25° by 0.25°, monthly	2003–2016	https://opendata.dwd.de/
Soil Moisture	CPC Soil Moisture V2	0.5° by 0.5°, monthly	2003–2016	https://psl.noaa.gov/data

2.2.1. GRACE Data

GRACE solutions are expressed by SHCs up to degrees/orders 60 or 96. The relation between spatial resolution and spherical harmonic coefficients can be approximately 20,000 km/L. so the GRACE RL-06 results can achieve a theoretical maximal spatial scale of 330 km or 220 km. However, post-processing may lead to no difference between the 60 and 96 degrees/orders of SHCs. We employed the SHCs with new 96 degrees/orders to ensure the TWS anomaly extraction in medium-scale regions. The newly released RL-06 models mainly come from three scientific centers: the Center for Space Research (CSR), Geo-Forschungs-Zentrum (GFZ) Potsdam, and Jet Propulsion Laboratory (JPL). All data sets can be obtained from the websites in Table 1. In this study, we adopt the RL-06 products with a maximal degree of 96 from CSR—the study period from January 2003 to December 2016 has 151 monthly solutions. Because of the influence of gravity satellite operations, 17 months of solutions are missing in the study period. Moreover, there is a gap of about 15 months between the GRACE and GRACE-FO missions. So, the time range for this research is selected as aforementioned for continuity. Although much research has been aimed at fixing the gap, it is beyond the scope of this study.

Following the general procedure, the C_{20} coefficient is replaced by independent measurement from satellite laser ranging (Technical Note TN-11) [41]. The degree 1 coefficients have been replaced by estimations using the method of Sun et al. (Technical Note TN-13) [42]. Next, the glacial isostatic adjustment (GIA) effect is removed with the method suggested by Geru A et al. due to the Dnieper River basin being located in an area influenced by the last glacial period [43].

2.2.2. Snow Water Equivalent and Soil Moisture from GLDAS and CPC

Snow water equivalent (SWE) and soil moisture (SM) derived from the Global Land Data Assimilation System model (GLDAS) are adopted to analyze the TWS change in the Dnieper River basin [44]. The Global Land and Data Assimilation System (GLDAS) was developed jointly by the National Aeronautics and Space Administration (NASA) Goddard Earth Science Data Information and Services Center (GES DISC) and National Oceanic and Atmospheric Administration (NOAA) National Center for Environmental Prediction (NCEP) [45]. Up to now, GLDAS has driven four land surface models (LSMs): Noah, Catchment (CLSM), the Community Land Model (CLM), and the Variable Infiltration Capacity (VIC). The data sets are organized as the spatial $1^\circ \times 1^\circ$ or $0.25^\circ \times 0.25^\circ$ resolution and 3-hourly, daily, and monthly temporal resolution separately [46,47]. In this article, we select the Noah datasets of version 2.1 from 2003 to 2016 with monthly time resolution and $1^\circ \times 1^\circ$ spatial resolution. The variates, including SM at a depth of 0 to 200 cm, SWE are used to simulate the TWS in the Dnieper River basin.

The Climate Prediction Center (CPC) Soil Moisture V2 data are used to simulate the TWS for validation. The CPC soil moisture data sets provide the monthly and daily global soil moisture data at the resolution of 0.5° from 1948 to the present [48,49]. The data sets are obtained by a land model, with the driving input fields including CPC monthly precipitation overland and global temperature from global reanalysis [50].

2.2.3. Total Water Storage from WGHM

The priori total water storage (TWS) information is needed as input when using the scaling method to restore the GRACE leakage effect described in Section 3.3. Here, the WaterGAP Global Hydrology Model standard version (WGHM 2.2d), a sub-model of the WaterGAP 2 model, is used to extract TWS anomalies. Excluding water in the glaciers, WGHM encompasses soil, snow, and canopy components in the vertical direction and lakes, reservoirs, wetlands, groundwater, and rivers in the lateral direction. The WGHM 2.2d has a time from 1901 to 2016, 0.5° spatial resolution, and monthly temporal resolution. The WGHM data are extracted and resampled as 1° by 1° grid data from 2003 to 2016 to compare with GRACE results [51].

2.2.4. Precipitation from GPCC

Usually, the TWS anomaly detected by GRACE is closely related to precipitation in the river basin. For analysis and verification, the precipitation in the Dnieper River basin from GPCC products is introduced. The precipitation data from the Global Precipitation Climatology Center (GPCC) are constructed based on 124,000 in situ measuring stations distributed worldwide [52]. All GPCC products are available in spatial resolutions of 1° , 0.5° , 0.25° , and 2.5° latitude and longitude, as well as the temporal resolution of the month [53]. In the paper, we adopt the data sets from 2003 to 2016 in 1° spatial resolution.

3. Methods

3.1. GRACE Data Processing

Generally, the gravity field of the Earth is expressed by the relation between geoid S and SH coefficients as in Equation (1),

$$S = R_e \sum_{l=0}^{\infty} \sum_{m=0}^l \bar{P}_{lm}(\cos\theta) [C_{lm}\cos(m\varphi) + S_{lm}\sin(m\varphi)] \quad (1)$$

where θ and φ are colatitude and longitude, R_e is the average radius of the Earth, $\bar{P}_{lm}(\cos\theta)$ is normalized associated Legendre function, and C_{lm} and S_{lm} are the SH coefficients provided by the GRACE RL-06 products.

The gravity changes could be inferred using the multiple monthly GRACE RL-06 harmonic coefficients. In other words, the mass transition with time within the Earth or above its surface is extracted. The harmonic coefficients from GSM files have already

removed the effect of the atmosphere, tides, and ocean. The remaining sources of time-variable mass changes are treated as a thin layer at the Earth's surface. Therefore, one can approximate the vertically integrated mass as a surface mass density $\Delta\sigma$ [2]. Equation (2), given by John Wahr, is adopted,

$$\Delta\sigma = \frac{R_e\rho_e}{3} \sum_{l=0}^{\infty} \sum_{m=0}^l \frac{(2l+1)}{(1+k_l)} \bar{P}_{lm}(\cos\theta) [\Delta C_{lm}\cos(m\varphi) + \Delta S_{lm}\sin(m\varphi)] \quad (2)$$

where ρ_e is the average density of the Earth, k_l are the load love numbers obtained from Han and Wahr [54], and $\Delta C_{lm}/\Delta S_{lm}$ are the variation in the coefficients. In practice, we convert $\Delta\sigma$ to equivalent water height (EWH) with the following equation:

$$\Delta H = \frac{R_e\rho_e}{3\rho_w} \sum_{l=0}^{\infty} \sum_{m=0}^l \frac{(2l+1)}{(1+k_l)} \bar{P}_{lm}(\cos\theta) [\Delta C_{lm}\cos(m\varphi) + \Delta S_{lm}\sin(m\varphi)] \quad (3)$$

A two-step filter strategy has been implemented in this paper, as the original GRACE signal includes the noise of high frequency and correlation. The south–north noise in the different odd and even high-degree coefficients for the same order has been first confirmed by Swenson and Wahr [4]. A method devised by Chen et al. in 2009 was used to suppress it [55]. The basic idea of this means is to suppose the fitted results are the correlation error. For the coefficients 6 and above, a polynomial of fourth order is constructed and fitted by the least square method. Then, the polynomial results are removed from corresponding spherical harmonic coefficients derived from GRACE observation. Next, to reduce the high-frequency noise, a Gaussian filter with a halfwave length of 300 km is applied following as Equation (4),

$$\Delta H = \frac{R_e\rho_e}{3\rho_w} \sum_{l=0}^{\infty} \sum_{m=0}^l \frac{(2l+1)}{(1+k_l)} \bar{P}_{lm}(\cos\theta) W_l [\Delta C_{lm}\cos(m\varphi) + \Delta S_{lm}\sin(m\varphi)] \quad (4)$$

where W_l are smoothing factor of Gaussian associated with degrees of harmonic coefficients.

A regional average kernel function ϑ is used to extract the Dnieper River basin mass change:

$$\vartheta(\theta, \lambda) = \begin{cases} 0, & \text{outside the basin} \\ 1, & \text{inside the basin} \end{cases} \quad (5)$$

Generally, ϑ is expanded as an SH function. According to the orthogonality of harmonic function, coefficients of ϑ , ϑ_{lm}^c , and ϑ_{lm}^s will be calculated and then employed for extracting the basin mass change, combining with Equation (6):

$$\overline{\Delta H} = \frac{R_e\rho_e}{3\rho_w} \sum_{l=0}^{\infty} \sum_{m=0}^l \frac{(2l+1)}{(1+k_l)} \bar{P}_{lm}(\cos\theta) W_l [\vartheta_{lm}^c \Delta C_{lm}\cos(m\varphi) + \vartheta_{lm}^s \Delta S_{lm}\sin(m\varphi)] \quad (6)$$

where $\overline{\Delta H}$ is the regional anomaly of EWH, and all other symbols in Equation (6) are the same as aforesaid. However, from the view of signal processing, the average kernel function is equal to a rectangular filter in the spectral domain, leading to signal leakage. The weighting function method, which is widely used in the digital signal processing domain, has been adopted to reduce the leakage caused by the sidelobe effect in the filter. Here, the weighting function is defined as a cosine function of latitude, and then the local mass changes can be obtained by Equation (7):

$$\overline{\Delta H} = \frac{\sum_{i=1}^n \Delta H_i \cos(\theta_i)}{\sum_{i=1}^n \cos(\theta_i)} \quad (7)$$

However, the signal has been damped due to spherical harmonic truncation and Gaussian spatial smoothing. This article uses forward modeling (FM), data-driven, and scaling methods to restore the GRACE observed signal.

3.2. Forward Modeling Approach

The constrained FM approach is utilized to correct the leakage error in the Dnieper River basin, and the following brief instructions are provided.

(1) We regard the GRACE observations as the initial mass anomalies fm_0 in the Dnieper River basin. That means the mass variation within the Dnieper River basin is defined as GRACE observations, and beyond the areas, it is considered zero.

(2) The initial mass anomalies are expanded to the SHCs at the degrees and orders 96. Then, a 300 km Gaussian filter and regional average kernel function are applied, the same as GRACE observations. Then, the forward model mass anomaly fm_1 is obtained.

(3) The residual between the GRACE observed mass anomaly and the forward modeling mass anomaly ($fm_g - fm_1$) is added to the initial mass anomaly. In previous studies, a scale factor of 1.2 is recommended, which can accelerate the convergence of the iteration, that is, $fm_0 = fm_0 + 1.2(fm_g - fm_1)$. Here, we choose 1.2 as the scale factor according to the data experiment. The new initial mass is repeated for the second step until the difference is less than a certain threshold or after a certain number of iterations. Unlike the large regions with apparent TWS variation, the number of iterations of the medium regions adjacent to weak TWS anomaly areas is smaller. In this research, we set the number of iterations to 20 according to the convergence curve depicted in Figure 2.

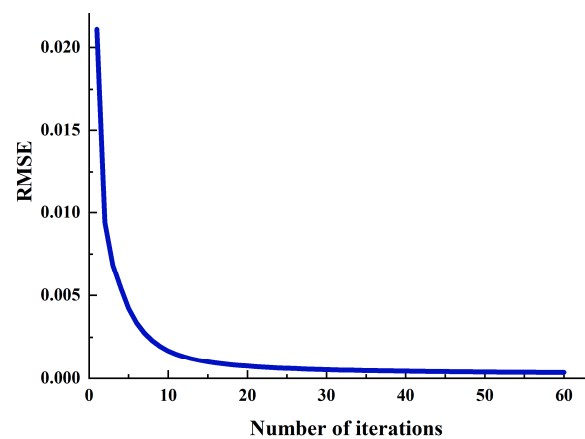


Figure 2. The convergence curve for the FM approach.

3.3. Scaling Approach

The scaling factor is critical for the scaling approach to recover the damped GRACE observation and depends on the prior hydrological model. The mass variation derived from hydrological models is considered the true mass variation in the river basin. The hydrological model is expanded in SH coefficients, truncated at degrees and orders 96, and smoothed by a 300 km Gaussian filter. The difference between the original hydrological model and the filtered is attributed to the leakage effect.

A single scaling factor for the Dnieper River basin is obtained by fitting the unfiltered model time series Δm_u and filtered time series Δm_f with the least square method, that is:

$$MIN = \sum (\Delta m_u - k \Delta m_f)^2 \quad (8)$$

where k is the scaling factor, and three single scaling factors are obtained by filtering the hydrological model GLDAS, CPC, and WGHM at the river basin scale.

Generally, TWS variation expressed by time series includes the terms of long trend and seasonal period as depicted in Figure 3. A reasonable approach is that the time series

of unfiltered and filtered models GLDAS, CPC, and WGHM are decomposed into long trend term, seasonal and residual components as Equation (9):

$$\Delta V_{total} = \Delta V_{long\ trend} + \Delta V_{seasonal} + \Delta V_{residual} \quad (9)$$

For this purpose, a least squares model fits the time series as Equation (10):

$$\Delta V_i = A + B\Delta t + \sum_{k=1}^n \alpha_k^c \cos\left(\frac{2\pi}{T_k} \Delta t\right) + \alpha_k^s \sin\left(\frac{2\pi}{T_k} \Delta t\right) + \varepsilon \quad (10)$$

where ΔV_i is the TWS anomaly averaging over the Dnieper River basin at the i month, A represents the TWS anomaly for the mean times, B is the long trend linear term, k is the numbers of periods, T_k is the period, α_k^c and α_k^s are the amplitudes of the cosine and sine terms of the same period T_k , and ε is the residual. Nevertheless, the periods T_k could not be determined directly from the time series of hydrological models.

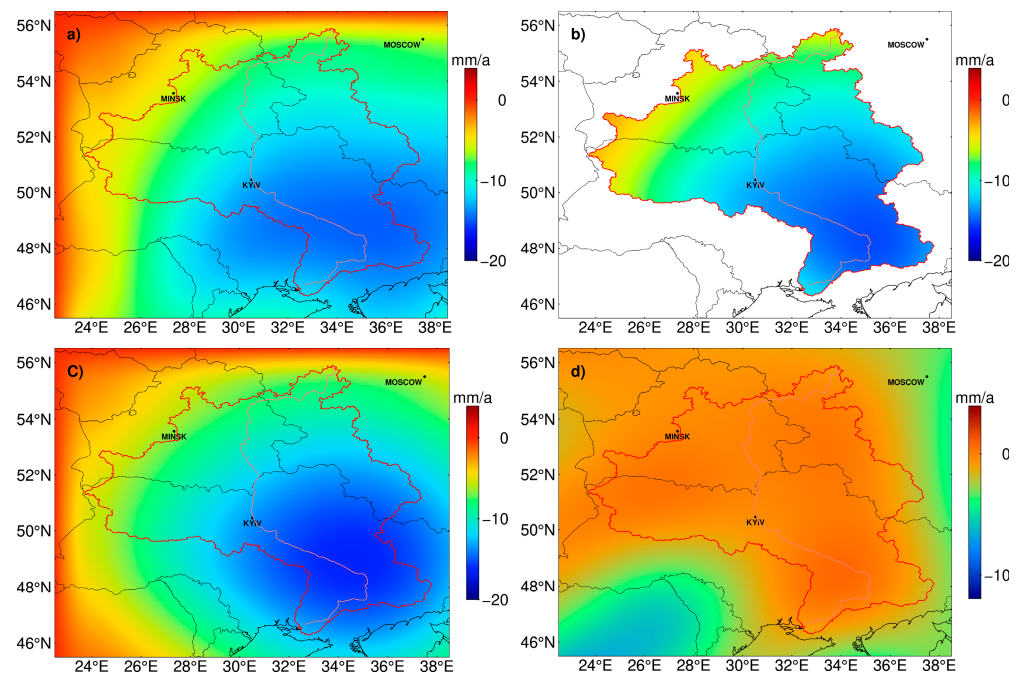


Figure 3. The trend of TWS anomaly from forward modeling (Unit: mm/a). (a) The GRACE observed mass rates of the Dnieper River basin from the results of GRACE observation with decorrelation and a 300 km Gaussian filter. (b) Forward modeling initial mass rates. (c) The mass rates are handled with the same filter approach as (a) computed from (b). (d) The difference in mass rate between (a) and (c).

3.4. Data-Driven Approach

In the time domain analysis, Vishwakarma has shown that the filtering process weakens the time series' amplitude and changes the phase [21]. There are two forms of data-driven approaches. One is the scaled form, which can be described as Equation (11):

$$\hat{F}_c = s(\bar{g}_c - \hat{l}_c) \quad (11)$$

where $\hat{F}_c$ is the corrected time series, $\bar{g}_c$ is the time series obtained from filtered GRACE spherical harmonic coefficient models, $\hat{l}_c$ is leakage obtained by two times phase shift, and s is the scale factor.

For Equation (11), $\bar{g}_c$ is obtained by the method described in Section 3.1. The scale factor s is calculated using Equation (12). We skip over the process of derivation and give the equation as,

$$s = \frac{\int_{\Omega} \vartheta(\theta, \lambda) d\Omega}{\int_{\Omega} \vartheta(\theta, \lambda) \bar{\vartheta}(\theta, \lambda) d\Omega} \quad (12)$$

where Ω denotes the surface of the Earth, $\vartheta(\theta, \lambda)$ is the kernel function, same as in Equation (5), $\bar{\vartheta}(\theta, \lambda)$ is the filtered kernel function. The scale factor s is independent of any other hydrological models.

For the leakages $\hat{l}_c$ calculation, we need to filter the GRACE field twice. The leakage time series $\bar{l}_c$ and $\bar{\bar{l}}_c$ are calculated by Equations (31) and (32), represented in Vishwakarma's paper [20]. Then, we shift the $\bar{\bar{l}}_c$ to $\bar{l}_c$ with the phase difference and calculate the mean ratio between them. Finally, we shift the $\bar{l}_c$ with the phase difference and multiply the mean ratio.

Another type of data-driven approach is called deviation data-driven. Unlike the scale data-driven approach, the modified approach introduced the deviation item instead of the scale factor. We give the method directly as,

$$\hat{f}_c = \bar{g}_c - \delta \bar{F}_c - \hat{l}_c \quad (13)$$

where $\delta \bar{F}_c$ is determined by $\frac{1}{A_c} \int_{\Omega} \delta \bar{F}(\theta, \lambda) \vartheta(\theta, \lambda) d\Omega$. More details about the scale and deviation data-driven approach can be found in Vishwakarma [21].

3.5. Uncertainty Estimates and Validation Method

For evaluating the relative efficiency of different approaches, several assessment indexes are applied to quantitatively analyze the uncertainty of estimates of TWS anomaly that are restored by FM, data-driven, and scaling approaches. The root mean square error (RMSE) is taken to assess the uncertainty of the restored GRACE-derived TWS anomaly, which is described as follows:

$$RMSE(\Delta S_R - \Delta S_T) = \sqrt{\frac{1}{n} \sum_{i=1}^n (\Delta S_R^i - \Delta S_T^i)^2} \quad (14)$$

where ΔS_R is the corrected time series derived from GRACE, ΔS_T is the time series of reference mass variation in a river basin, and n is the number of months in the research period. In practice, we propose to use the MASCON products released by CSR as the reference mass variation (<http://www2.csr.utexas.edu/grace>, accessed on 12 April 2024) [56]. Compared to the unconstrained SH solutions, the mascon solutions avoid attenuating the signals by post-processing. An RMSE close to zero indicates excellent agreement between the restored and true values.

Like the RMSE method, Nash–Sutcliffe Efficiency (NSE) is often used to evaluate the performance of approaches:

$$NSE = 1 - \frac{\sum_{i=1}^n (\Delta S_R^i - \Delta S_T^i)^2}{\sum_{i=1}^n (\Delta S_T^i - \overline{\Delta S_T^i})^2} \quad (15)$$

where $\overline{\Delta S_T^i}$ is the mean of the true value, and other symbols are the same as above. An NSE value close to 1 means excellent performance for the corrected results.

3.6. Cross Wavelet Transform

A time-frequency method is specially introduced to validate the components of seasonal variation from the results simulated by hydrological models, that is, the cross wavelet transform (XWT). XWT was first devised by A. Grinsted et al., and the basic idea is to examine two time series together in the time-frequency domain to extract the features of

trends or periodicities [57]. The XWT was applied to the time series of GRACE observation, and the one was simulated using hydrological models. Then, one could examine whether a region with a significant common power and a consistent phase relationship exists. This region may illustrate and validate the climate variability derived from GRACE. XWT is constructed by two continual wavelet transforms given the CWT results of two time series derived from GRACE and hydrological models.

4. Results

As mentioned in Section 2, four approaches combined with three hydrological models reduce the leakage error. We show the corrected results as two groups according to the model properties. One is the auxiliary model-independent approach, including the FM and data-driven approaches, and another is the dependent type containing the single and multiple factor approaches.

4.1. Results of Model-Independent Approach

We represent the TWS change in Figures 3–5 and the performance in Table 2, which is inversely by the model-independent approaches, including the FM and data-driven approaches.

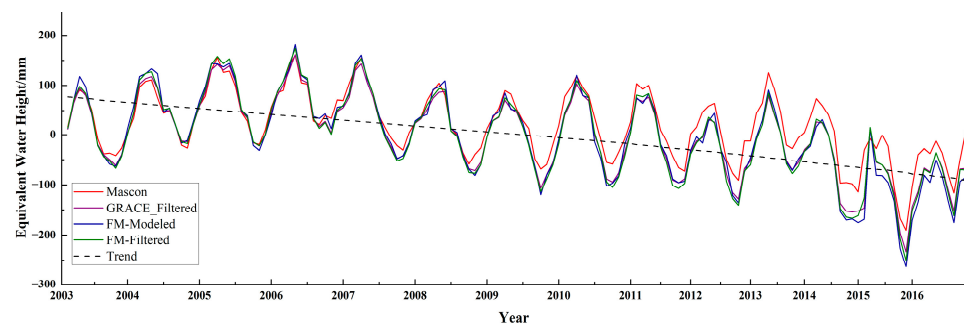


Figure 4. GRACE time series of TWS anomaly that has been conducted with decorrelation and Gaussian filter (blue), Mascon time series (red) extracted from CSR RL06 Mascon Solutions (version 02), forward modeling (FM) ‘true’ time series modeled by a 10-iteration procedure (green), and forward modeling ‘true’ time series filtered with the same filters of GRACE (purple), the residuals time series between recovered and ‘true’ time series.

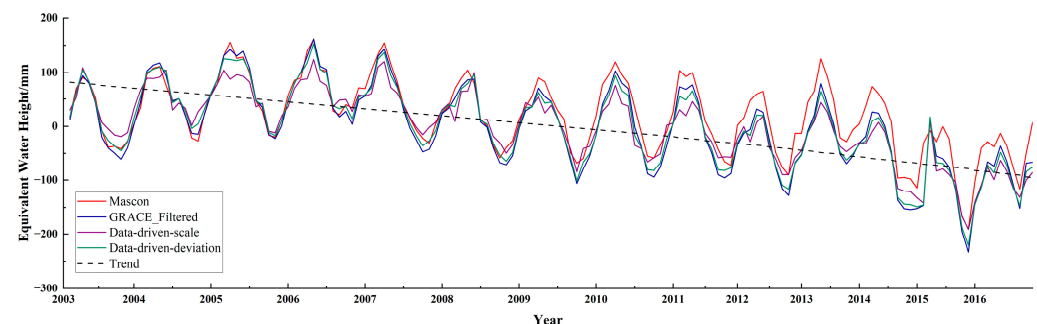


Figure 5. GRACE time series of total water storage that has been conducted with decorrelation and Gaussian filter (purple), Mascon time series (red) extracted from CSR RL06 Mascon Solutions (version 02), forward modeling (FM) ‘true’ time series modeled by a 50-iteration procedure (green), and forward modeling ‘true’ time series filtered with the same filters of GRACE (purple), the residuals time series between.

Table 2. Comparison of the Mascon time series and the reconstructed time series derived from the different recovered approaches.

Model	FM			Data-Driven				SF			MF				
	R	NSE	R	NSE	k	R	NSE	K	R	NSE	K1	K2	K3	R	NSE
—	3.04	0.796	3.40	0.745	1.33	3.98	0.651	—	—	—	—	—	—	—	—
WGHM	—	—	—	—	—	—	—	1.073	3.33	0.756	1.23	1.02	—	3.74	0.692
GLDAS	—	—	—	—	—	—	—	1.072	3.32	0.757	1.11	1.06	—	3.36	0.751
CPC	—	—	—	—	—	—	—	1.082	3.37	0.75	1.02	1.04	1.14	3.11	0.787

Note. R denotes the RMSE errors (Unit: cm), NSE is Nash–Sutcliffe efficiency, k is the scale factor, and k1, k2, and k3 are the scaling factors for trend, annual and semiannual items.

4.1.1. Convergency of Forward Modeling Approach

Figure 3 shows the trend of TWS anomaly recovered by the FM approach described in Section 3.2 in the spatial domain. Comparing the (a) and (b) in Figure 3, the declined source of mass change rate after 10 iterations of the FM approach is more concentrated in the south of the Dnieper River basin. After the filtering process that is the same as that of GRACE, the recovered mass rate (c) is -12 ± 1.44 mm/a, close to the initial mass rate (a). Though (a) and (c) have the characteristic of boundaries both at the values of -5 mm/a and -10 mm/a, those forms of expression vary. For Figure 3a, the mass rate changes in a fan region formed by the boundary, while for Figure 3c, the mass rate varies in ring regions formed by the boundaries. In Figure 3c, boundaries tend to converge. In other words, the leakage error effect is converged behind the FM approach's correction. The residuals between the initial mass rate and the filtered mass rate are depicted in (d) of Figure 3 to analyze the effect of the FM approach. As (d) shows, most of the region in the Dnieper River basin has mass rates close to zero. According to the features of convergence and residuals, we may reasonably confirm that the leakage effect influenced the south region of the Dnieper River basin. The main reason is a long TWS decline combined with the weak TWS variation region, the Black Sea, adjacent to the south of the Dnieper River basin.

Figure 4 shows the time series of the TWS anomaly corrected by the FM approach in the Dnieper River basin from 2003 to 2016. In contrast to the time series derived from CSR Mascon products, the corrected time series has a fine consistency. All the results represent the same variation trend. The TWS anomaly exhibits a rising trend from 2003 to 2006 and represents a declining trend for the rest of the research period. During the increasing period, the main post-processing error represented leakage in, while during the declining period, it represented leakage out. If we examine the efficiency of the FM approach for two parts at the demarcation point of 2006, the deficiency of the FM method may be revealed. From 2003 to 2006, the difference between the corrected and Mascon time series was magnified. In other words, the FM method increases the trend of separation between filtered time series and 'true' time series. After 2006, the corrected time series is closer to the 'true' time series. The FM method property may cause this phenomenon because it is more sensitive to the time series trend. That is to say, during the increasing period, the FM method magnifies the increasing trend and vice versa.

4.1.2. Phase Shift Error Caused by Data-Driven Method

In addition to the FM method, two data-driven approaches have been conducted for the same river basin. Figure 5 shows the results recovered by two forms of data-driven approach in the time domain. Although all of the time series show a similar fluctuation, two abnormalities exist. First, both forms have relatively abnormal peaks in the spring of 2005, 2011, and 2015. The reason for this may be the influence of the data-driven approach. A critical step for the data-driven approach's processing procedure is the phase difference calculation for the filtered time series. Examining the filtered time series, the characteristic of bimodal distribution is manifested in the spring of 2005, 2011, and 2015. When calculating the phase difference of the filtered time series, the bimodal distribution could be distorted by the results as a phase shift. For instance, the peak of the time series corrected by the scale

data-driven approach in the spring of 2005 shifted nearly 2 months ahead of the ‘true’ one. The last abnormality is that the amplitudes corrected by the two forms of the data-driven method are lower than those of the filtered GRACE one. Vishwakarma et al. defined leakage as the contribution from the signal outside the region of interest and corrected the time series subject to leakage error using a scale factor and a leakage time series [20]. The scale factor is obtained by taking a ratio between the filtered and twice-filtered regional averaged signal and represents a true attenuation caused by the filter only for the region of interest and surrounded by similar hydrological signal strength. Unfortunately, the regions surrounding the Dnieper River basin hold totally different hydrological processes, such as the Black Sea and the Wisla River basin. Furthermore, the leakage time series is subtracted from the filtered GRACE one before multiplying the scale factor. Combined with the above analysis, the amplitudes of the TWS anomaly time series recovered by the data-driven method in the Dnieper River basin are lower than the filtered GRACE time series.

4.1.3. Comparison of Model-Independent Approaches

The uncertainty estimates of two kinds of independent approaches by the means are described in Section 3.5 and shown in Table 2. The FM approach performs best with 3.04 RMSE and 0.796 NSE, respectively. The rest of the independent approaches have almost equal capability to weaken the effects of leakage. Particularly, we will give more detail about the scale data-driven approach. From Table 2, the results repaired by the scale data-driven approach are the worst in terms of RMSE and NSE. Compared with the deviation data-driven approach, the magnifying process calculated by multiplying the scaling factor k magnified the attenuated amplitude and residual errors simultaneously. It is important to note that the scaling factor k in the scale data-driven method only depends on the regional kernel function. That is to say, the scale data-driven approach is independent of any auxiliary hydrological or meteorological models. Based on the above analysis, the FM approach is more accurate for repairing damaged signals caused by filtering in the three model-independent approaches.

4.2. Results of Model-Dependent Method

Like Section 4.1, the TWS anomalies inversed by single and multiple scaling factor approaches are shown in Figures 6–10.

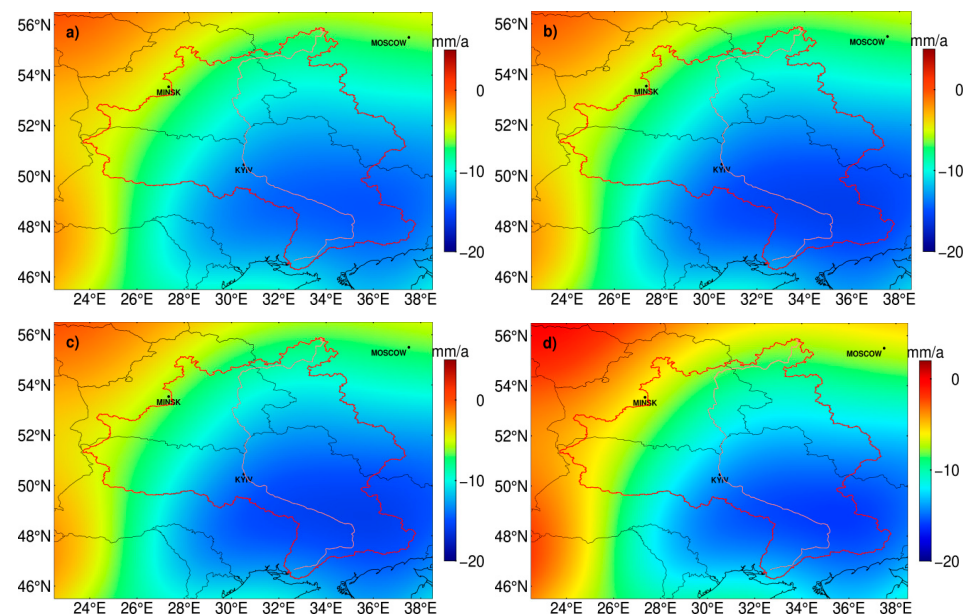


Figure 6. The trend of TWS anomaly. (a) is GRACE-filtered results, (b) is the results recovered by the single factor derived from WGHM, (c) is the results recovered by the single factor derived from GLDAS, (d) is the results recovered by the single factor derived from CPC.

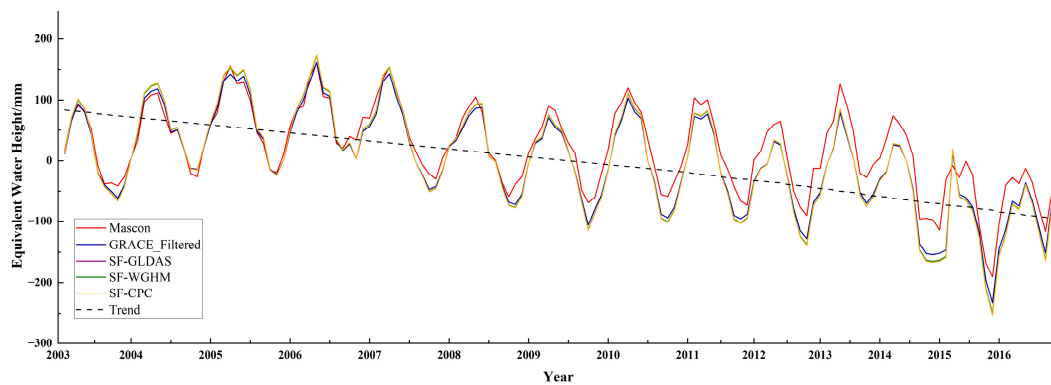


Figure 7. The time series of TWS anomaly recovered by single factor approach, the ‘true’ time series for validation obtained from CSR MASCON products (red), the time series after the filter process, the time series recovered by a scaling factor calculated from the WGHM (green), and GLDAS (blue), and CPC (orange) models.

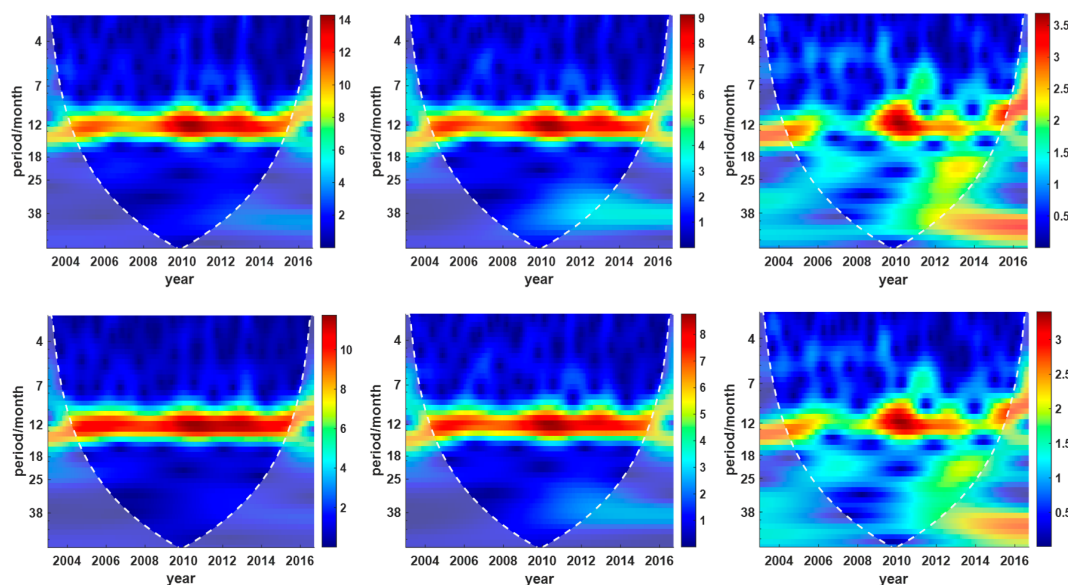


Figure 8. The XWT of time series between GRACE time series of TWS anomaly and three-time series of TWS anomaly simulated from hydrological models. The first row is the results of XWT that GRACE filtered time series with unfiltered time series derived from WGHM, GLDAS, and CPC models; the second row is the results of XWT that GRACE filtered time series with filtered time series derived from WGHM, GLDAS, and CPC models.

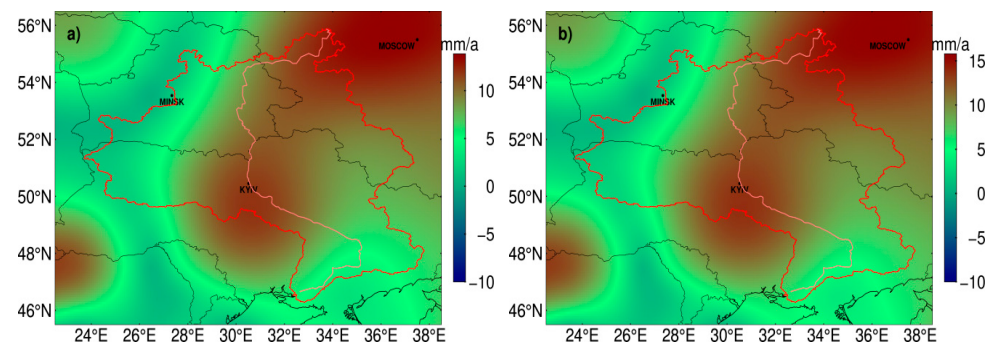


Figure 9. A multiple factor approach corrected the semi-annual amplitude variation in TWS anomaly in the Dnieper River basin. (a) The semi-annual amplitude variation in TWS anomaly separated from the filtered GRACE results, (b) the one corrected by multiple factor approach based on (a).

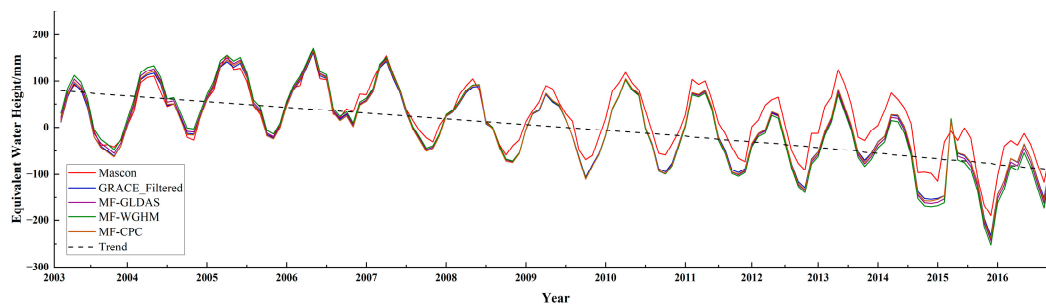


Figure 10. The time series of TWS anomaly in the Dnieper River basin for multiple scaling factor approach.

4.2.1. Inefficiency for Multiple Trends by Single Scaling Factor Approach

Corresponding to model-independent approaches, two model-dependent approaches are implemented in this article: single and multiple scaling factor approaches. Following the method described in Section 3.3, the restrained signal derived from GRACE products is restored and depicted in Figures 7–10.

In Figure 6, the recovered trend of TWS anomaly by the single factors calculated from three hydrological models holds a similar variation pattern. The TWS anomaly is decreasing from northwest to southeast, which agrees with the feature of the climate of the Dnieper River basin. There is almost no distinction between filtered results (a) and corrected results (b) and (c). Those trends follow the scaling factors 1.073 and 1.072 calculated from the hydrological model WGHM and GLDAS. It is implied that both WGHM and GLDAS are less sensitive to the Dnieper River basin. Compared with Figure 6a, the trend of TWS anomaly in Figure 6d has been enhanced visibly. The TWS change rate has been recovered from -12 ± 1.44 mm/a to -13 ± 1.56 mm/a with the single factor 1.082 derived from the CPC soil moisture model. Despite the consequence of (d) in Figure 6 possessing an apparent variation, there is no evidence to confirm that it is relatively more effective in leakage error repair. Further analysis of the efficiency of the single factor approach will be conducted in the time domain.

In Figure 7, the TWS anomalies corrected by the single factor approach, derived from the hydrological model GLDAS and WGHM, are barely seen. This situation is in agreement with the trend depicted in the spatial domain. Like the FM method, the time series in Figure 7 is divided into two parts in 2006. From 2003 to 2006, all corrected time series are away from the ‘true’ time series relative to the filtered one. From 2007 to 2016, the corrected time series are close to the ‘true’ time series. This phenomenon existed in both Figures 6 and 7, implying that the corrected trend term dominates the results recovered by the single factor approach. All the results mentioned above depicted in both spatial and time domains seem to suggest the best one is corrected by a scaling factor of 1.082 derived from the CPC model. On the contrary, the more proper results are obtained by the single factor 1.072 calculated from the GLDAS model from the view of RMSE and NSE. In other words, the efficiency of the single factor approach is opposite to the value of the scaling factor. This state of affairs reveals that the main portion of leakage error caused by the filtering process is not all from the trend term for the Dnieper River basin. Hence, the annual and semi-annual terms of TWS anomaly also need to be considered apart from the trend term.

4.2.2. The Period Determination by Cross Wavelet Transform

Generally, the calculation of multiple scaling factors assumes that the time series of TWS anomaly simulated by models can be decomposed into trend, annual, and semi-annual terms. In practice, there is no explicit evidence to support that assumption. This article employs the XWT method to investigate the periodical relatives between the filtered GRACE time series and the one simulated by hydrological models. The XWT results are shown in Figure 8, presented by the time and frequency domain. Compared with the

first row in Figure 8, there are no changes in the periodic property in the second row. That is to say, the filtered process attenuated the signal energy but did not influence the periodical property. It is explicit that the peak of power in the first and second columns is approximately concentrated over the annual cycle. The third column includes a power sub-peak in the semi-annual cycle. Then, conclusions could be made that the trend and annual scaling factors can be calculated from the WGHM and GLDAS models. The semi-annual scaling factor can be derived from the CPC model except for the trend and annual one. The scaling factors are listed in Table 2.

4.2.3. The Semi-Annual Cycle Variation in TWS Anomaly Extracted by Multiple Scaling Factor Method

According to the XWT, we have calculated the multiple scaling factors using the WGHM, GLDAS, and CPC models, respectively. As listed in Table 2, the performance of RMSE and NSE is inversely proportional to the scaling factors of the trend term, which is identical to the analysis in the single factor method. There is no apparent difference between the three corrected annual amplitude variations because all scaling factors of the annual term listed in Table 2 are close to 1. Hence, the semi-annual amplitude variation in the Dnieper River basin is concerned only and exhibited in Figure 9. Almost all of the semi-annual changes of TWS anomaly are positive, and the maximum variation is located in the middle and lower reaches of the Dnieper River basin. The most reasonable region of maximum variation may be located upstream of the Dnieper River basin, according to the features of the continental climate. The reason for this contradictory situation may be the effect of water redistribution in that the reservoirs and irrigated farmland are mainly set in the middle and lower reaches. Compared with (a), the area enclosed by fluorescent green in (b) is narrowing obviously, which implies that semi-annual amplitude changes have been enhanced. The difference in the color bars in (a) and (b) needs to be noted.

The time series in Figure 10 were disposed of as in Section 4.1 again for analyzing the efficiency of the multiple factor approach based on three hydrological models. From 2003 to 2006, the phase shift caused by the phase difference calculation of the data-driven approach is not seen. However, the trend of separation between the ‘true’ time series and the ones corrected by the WGHM and GLDAS models is also apparent. This anomaly results from the conclusion that the leakage error does not mainly come from the trend term. For the rest, the time series, including filtered and recovered, appear in fine agreement with the ‘true’ time series. The semi-annual term is magnified maximally with the factor 1.14, compared with the rest of the seasonal terms derived from CPC models. The results indicate that the leakage error comes mainly from the semi-annual term of TWS anomaly.

4.3. Climate Features and Snowmelt States in Dnieper River Basin

To further investigate the climate insight behind the TWS anomaly, the relations between the filtered GRACE results and the one derived from the CPC model have been depicted in Figure 11. It appears strong seasonal fluctuation in the TWS anomaly is derived from the GRACE and CPC model. The value of the TWS anomaly attained a maximum and minimum every March and October, respectively. Furthermore, there is a trend of decline in the TWS anomaly from northwest to southeast in the Dnieper River basin. GRACE has revealed continental climate features from the perspectives of both the spatial and time domains. The peaks of GRACE TWS anomaly are usually logged behind the maximum TWS of the CPC model for approximately 1 month. This suggests that it takes about a month for the GRACE response to reflect the results of the CPC model. The inverted results by GRACE include components of water balance such as soil moisture, surface water, ice or snow, biosphere, and groundwater. Nevertheless, soil moisture is the only component of the CPC model. Concerning the amplitude, it is lower for CPC than GRACE.

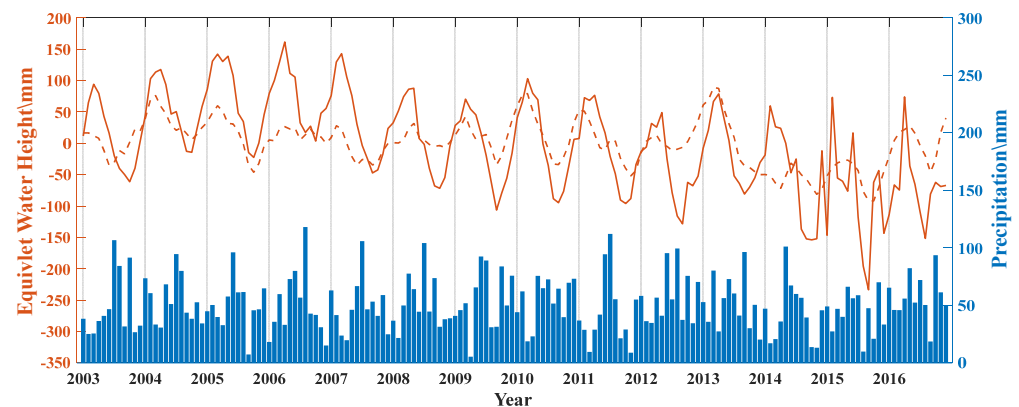


Figure 11. The correlation of TWS anomaly between the obtained GRACE (solid line), CPC (dash line), and GPCC (bar).

In addition to the hydrological model CPC, it is feasible to introduce the climatological model GPCC to explore the hydrological process together. At first sight, there is no apparent correlation between the precipitation anomaly extracted from the GPCC model and the TWS anomaly derived from the GRACE or CPC model. Even there is a common abnormal situation every year that the maximum precipitation is in summer or autumn, while the peaks of TWS anomaly are in spring. The snowmelt may be critical to understanding this abnormality, considering the characteristics of climate in the Dnieper River basin. Usually, it has little impact on the hydrological process in low-latitude regions. However, the Dnieper River basin is located in the middle latitude and holds a long period of low temperature from November to February of the next year. The snow could be preserved in a low-temperature period and begin melting every March. Except for runoff, the snowmelt is converted to soil moisture by osmosis. It may be a reasonable interpretation of the property of seasonal variation expressed by GRACE in the time-spatial domain. In conclusion, snowmelt is the primary water resource for the Dnieper River basin.

4.4. Extreme Temperature Impacts in Dnieper River Basin

Making a general view of all data experiments, the common, more significant deviation existed in 2015, which has not been discussed and interpreted. It needs to be emphasized that the time series of GRACE in Figure 11 is obtained by interpolation for the data of missing months to match with the time of the CPC. As mentioned above, the situation in 2015 is within the period of declination of TWS anomaly. This case and the trend of decline are also analyzed together in terms of temperature. The temperature anomaly of February is shown in the spatial domain, considering the peaks that appear every year and the alternating months of winter and spring. From Figure 12, the temperature anomaly approaches or falls below 0 °C from 2003 to 2007 and 2010 to 2012 and above 0 °C from 2008 to 2009 and 2013 to 2016 in the Dnieper River basin. The variations in temperature anomaly relative to the long-term mean of February from 2003 to 2016 influences the TWS anomaly by the mechanism that high temperature leads to snowmelt and increased runoff and evaporation. According to the water balance equation, the temperature effects propagate to TWS change, representing an increasing or decreasing trend that is contrary to temperature anomaly. Therefore, it is reliable to consider the TWS anomaly decreasing trend derived from GRACE data sets influenced by the temperature to a certain extent.

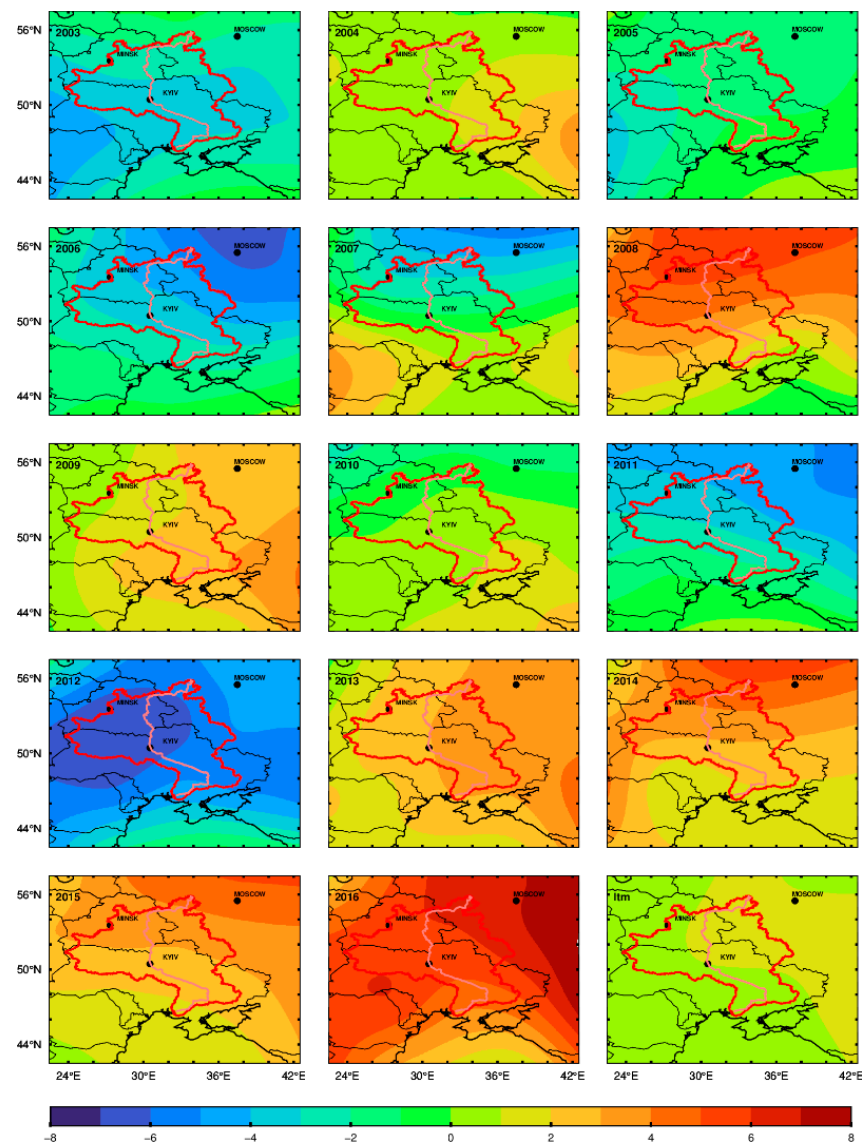


Figure 12. The temperature anomaly and long-term mean of every February from 2003 to 2016 in the spatial domain (unit: deg C). The last panel is the long-term mean over the period.

Besides the declining trend, an extreme situation existed in the minimum valley value in September 2015 that may have been caused by climate change. The study conducted by Pokhrel et al. suggests that a decrease in TWS may increase the risk of drought in the future [58]. As reported by Henny et al., Europe, particularly central and eastern Europe, has experienced a prolonged drought from summer to early autumn [59]. According to Figure 13, the temperature in August 2015 was more than 3 °C, which is higher than the seasonal mean. Moreover, the rainfall in the Dnieper River basin was relatively low in the same month. As a result, the minimum precipitation would be found in August 2015 and detected by the GRACE in September, caused by the propagation delay from precipitation to GRACE. Since August 2015, the precipitation has been increasing, while the TWS trend detected by GRACE holds a less obvious increase immediately. The reason for this may be the ‘legacy effects’ proposed by Anderegg et al. [60]. The water-holding capacity in the Dnieper River basin has not completely recovered from the extreme climate.

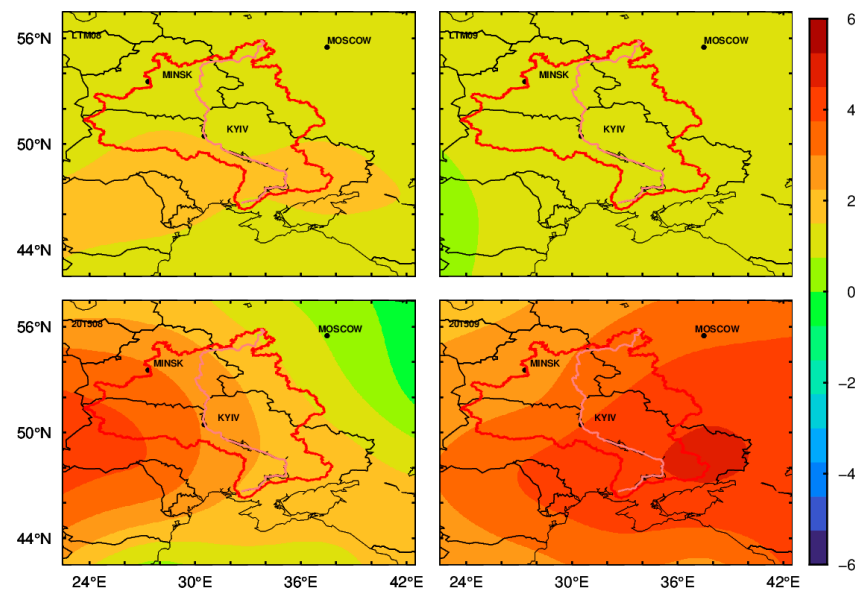


Figure 13. The temperature anomaly and long-term mean of August and September 2015 in the spatial domain (unit: deg C). The first row of the figure is the long-term mean temperature in August and September, and the last row is the corresponding monthly temperature anomaly in 2015.

Turning attention to the peaks from GRACE in 2015, the snowmelt appeared and transformed to soil moisture before winter was over, which arose from the temperature anomaly rise of February in Figure 12. The TWS anomaly from GRACE approached the maximum in March or April, and held a subpeak in February, which was the same as shown in 2011 or 2012. However, there was only a peak in February 2015. Regarding the subpeak in June, we do not discuss it more, as it is obtained by interpolation. From the perspective of mathematics, the filtering process is a weighted average process performed in the frequency domain described in Section 3.1. The signal outside the study region will be aliased into the Dnieper River basin if the signal inside is relatively weak. Considering the drought state of 2015, the variation in TWS is the minimum at the year's level in the study period. Therefore, the deviation is likely to be caused by the influence of the filtering process and the relatively low signal power in the Dnieper River basin in 2015.

5. Conclusions

Although the observations provided by GRACE have been used to explore and monitor the TWS anomaly at the global or regional scale, few discussions have focused on a medium-scale river basin close to a weak signal area.

This paper investigates the TWS anomaly in the Dnieper River basin, where the medium river basin is located near weak signal areas. Initially, we tested two types of inversion approaches to obtain a reliable TWS anomaly through a series of data experiments with GRACE Level2 products. We then analyzed the inversion results in the spatial and time domain and compared them with those extracted from Mascon products to verify their reliability (Sections 4.1 and 4.2). Subsequently, we combined the TWS anomaly derived from GRACE with other meteorological and hydrological models to gain insights into the anomaly (Section 4.3). Finally, we discussed and analyzed the deviation and extremely low variation observed in 2015. The main conclusions of this article are as follows:

1. Based on a numerical study of model-independent approaches, it can be concluded that (a) the FM method is more sensitive to the TWS anomaly trend term and makes the trend variation converge at a ± 10 mm/a. Through a comprehensive analysis, the FM approach achieves the best TWS anomaly inversion in terms of 3.04 RMSE and 0.796 NSE. Furthermore, by analyzing the results recovered by the FM approach in spatial and time domains, the south region of the Dnieper River basin was found to be more sensitive to the adjacent area of weak TWS variation. (b) The data-driven approach is characterized

by a phenomenon of phase shift that appeared in the years with double peaks in the time domain, which distorted the corrected results. Additionally, the data-driven approach is unsuitable for recovering leakage errors in medium-scale regions surrounded by different hydrological signal strengths.

2. Numerical tests for model-dependent approaches show that (a) the single scaling factor approach is unsuitable for repairing the leakage error with multiple trends simultaneously. (b) Combined with the resulting analysis of the single factor method, the multiple scaling factor method confirms that the primary resource of leakage error is from semi-annual terms rather than the trend and annual terms in the TWS of the Dnieper River basin. Furthermore, the XWT transform method determines the periodic terms based on the time-frequency domain instead of empirical assumptions.

3. GRACE observations shown in the spatial domain are consistent with the climatic features of the Dnieper River basin, namely that the continental climate is gradually more significant from the northwest to the southeast. The snowmelt is the primary source of TWS of the Dnieper River basin, as shown by analyzing the variation in GRACE observations, the regional temperature, precipitation, and the catchment area. The temperature changes also lead to the trend changes in TWS anomaly over the research period. Moreover, the response time for GRACE to precipitation is approximately a month or two in the warm period and four or five months in the cold period.

4. The most considerable discrepancy between the GRACE observation and Mascon results is caused by the mechanism of filter calculation in the frequency domain, coupled with the drought event that occurred in 2015. The delayed recovery in water-holding capability was detected by the GRACE TWS anomaly after August 2015.

Although the FM approach obtained relatively good results in this work, limitations also need to be noted. The FM approach is more sensitive to trend terms and depends on experience in determining the acceleration factor. Moreover, the scale approaches depend on the hydrological model, which may add uncertainty to the recovered results.

Author Contributions: Conceptualization, T.Z. and W.L.; software, T.Z. and W.L.; Writing—original draft, T.Z.; validation, T.Z., B.J., J.Y. and S.B.; formal analysis, T.Z. and J.Z.; writing—review and editing, S.B. and B.J. All authors have read and agreed to the published version of the manuscript.

Funding: This research was funded by the National Natural Science Foundation of China (no. 41971416, 42122025) and the Shandong Province Natural Science Foundation (no. ZR2022QD025).

Data Availability Statement: The datasets analyzed in this study are listed in Table 1.

Acknowledgments: All authors gratefully acknowledge the Center for Space Research at the University of Texas, Hannes Müller Schmied, NOAA PSL, the German Meteorological Service, and NASA for providing GRACE data, WGHM model outputs, CPC Soil Moisture V2 model, GPCC full monthly precipitation data, and GLDAS land surface model.

Conflicts of Interest: The authors declare no conflicts of interest.

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