



- An improved GRACE-derived groundwater storage
- anomaly (igGWSA) dataset over global land with full
- 3 consideration of non-groundwater components based on
- 4 current new datasets
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- 12 Abstract: Accurate quantification of global groundwater storage anomaly (GWSA) is imperative for 13 global water security and socio-economic sustainability. The Gravity Recovery and Climate Experiment (GRACE) satellite has emerged as a prevailing methodology for estimating GWSA. 14 However, oversimplification of non-groundwater components potentially compromised its accuracy in 15 most previous studies. Here we present an improved GRACE-derived GWSA dataset at the global scale, 16 17 namely igGWSA, with full consideration of non-groundwater components including glaciers, snow, permafrost, lakes, reservoirs, surface runoff, profile soil moisture (PSM), and plant canopy water based 18 on current new datasets. In particular, PSM was generated based on Catchment Land Surface Model 19 20 and random forest algorithm. igGWSA demonstrated strong agreement with well-observed groundwater level and model-simulated GWSA in five globally recognized hotspots of groundwater 21 depletion. Compared to igGWSA with full consideration, simplified estimation would lead to 22 23 misinterpretations of groundwater storage variations in glacier-covered regions, giant lakes, and 24 deep-soil areas, highlighting the necessity of comprehensively accounting for non-groundwater 25 components in estimating GWSA, especially under a changing environment. igGWSA dataset is publicly available on Zenodo through https://doi.org/10.5281/zenodo.16871689 (Wang et al., 2025). 26

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1. Introduction

hydrological component in global terrestrial water cycle (Adams et al., 2022). Groundwater is a fundamental source of drinking water and agricultural irrigation, with 38% of global area equipped for irrigation relying on groundwater (Siebert et al., 2010). Groundwater-dependent ecosystems (GDEs) are identified worldwide (Link et al., 2023) and are found to be closely associated with biodiversity hotspots across global drylands (Rohde et al., 2024). Therefore, groundwater is of great significance for achieving the sustainable development goals (SDGs) proposed by the United Nations, such as No Poverty (SDG 1), Zero Hunger (SDG 2), Clean Water and Sanitation (SDG 6), Climate Action (SDG 13), and Life on Land (SDG 15) (Gleeson et al., 2020). However, climate change has imposed profound impacts on the atmosphere, hydrosphere and cryosphere (Prein and Heymsfield, 2020; Su et al., 2022; Ombadi et al., 2023), and particularly triggered changes in groundwater storage (GWS) through altering water supply-demand balance and groundwater recharge (Taylor et al., 2013; Condon et al., 2020; Kuang et al., 2024). Moreover, intensified anthropogenic activities (e.g., groundwater withdrawals for irrigation) have led to global groundwater depletion (Wada et al., 2010; De Graaf et al., 2017), which left vast populations threatened by unsustainable groundwater resources (Gleeson et al., 2012) and gave rise to eco-environmental issues such as land subsidence (Hasan et al., 2023) and river baseflow reduction (De Graaf et al., 2024). Therefore, accurate and quantitative monitoring of GWS variations is essential for ensuring global water security, food security, and socio-economic sustainability. Conventional monitoring of groundwater dynamics primarily depends on well-based observations. Despite the high reliability, the availability of such data remains severely constrained by economic costs, spatial accessibility, and data sharing policies (Adams et al., 2022). Consequently, related studies are typically conducted at local to regional scales, whereas large-scale and particularly global-scale analyses remain critically underexplored (Fan et al., 2013; Berghuijs et al., 2022; Jasechko et al., 2024). Notably, all these few large-scale studies suffer from spatial underrepresentation due to the extremely uneven distribution of monitoring wells. Moreover, point-scale measurements fail to delineate spatially continuous groundwater dynamics, nor can they adequately capture the heterogeneity of 2

Constituting the Earth's largest reservoir of liquid freshwater, groundwater serves as a critical





56 spatial limitations of in situ observations. Nevertheless, the reliability of model-simulated groundwater 57 dynamics is subject to other limitations. For example, the accuracy of simulations is sensitive to quality 58 of forcing data and inherent uncertainties in model structure (Döll and Fiedler, 2008; Berghuijs et al., 59 2022). Besides, owing to the absence of human activity module, many models capture only natural 60 variability patterns without accounting for the effects of human-induced hydrological processes such as 61 groundwater abstraction and irrigation practices (Fan et al., 2013; Pokhrel et al., 2021). In addition, the 62 vertical representation of aquifer systems in some models is too simplified to reliably simulate the 63 evolution of GWS (Gascoin et al., 2009). In 2002, the Gravity Recovery and Climate Experiment (GRACE) satellite was launched jointly by 64 65 the National Aeronautics and Space Administration (NASA) and Deutsches Zentrum für Luft- und 66 Raumfahrt (DLR) (Tapley et al., 2004a). GRACE mission has created unprecedented opportunities for 67 detecting terrestrial mass redistribution and provided an innovative perspective to quantify GWS variations (Tapley et al., 2004b). Changes in GWS can be isolated from changes in GRACE-detected 68 69 terrestrial water storage (TWS) by removing other non-groundwater components (Rodell et al., 2009). 70 Compared to in situ observations and model simulations, GRACE-based estimation demonstrates 71 distinct superiority. Horizontally, the global coverage of GRACE enables continuous monitoring of 72 large-scale groundwater variations. Vertically, GRACE-derived groundwater storage anomaly (GWSA) 73 represents the integrated dynamics of aquifer systems, providing more holistic characterization than 74 monitoring wells or predictions of hydrological models. 75 Although GRACE has emerged as a prevailing methodology for GWS estimation, limitations still remain in current GRACE-based studies. On the one hand, TWS is the summation of GWS and 76 77 non-groundwater storage. The more comprehensively non-groundwater components are taken into 78 account, the more accurate the separated GWS information will be. However, non-groundwater 79 components considered in most previous studies only encompass soil moisture, snow, plant canopy 80 water, and surface runoff (Table S1), which may be applicable to areas with limited types of water 81 bodies. For areas characterized by complicated hydrological systems (e.g., coexisting glaciers, 82 permafrost, and lakes), such ignorance will erroneously attribute the signals of unaccounted

hydrogeological characteristics. Hydrological models provide an alternative approach to address the





84 estimation. Among the neglected components, glaciers typically exhibit the most pronounced 85 magnitude of mass change. Therefore, the potential impact of incomprehensive consideration on 86 GWSA estimation is expected to be the greatest in glacier-covered regions. Due to the absence of glacier module in most land surface models (LSMs) and hydrological models, glacier mass balance 87 88 cannot be obtained from model simulations as other components. To our knowledge, the vast majority 89 of previous studies conducted in glacier-covered regions worldwide fail to take into account glacier 90 water storage when estimating GWSA (Table S1). 91 On the other hand, although soil moisture storage is involved in most previous studies (Table S1), 92 the adopted soil moisture data characterize water content within fixed-depth soil layers only instead of 93 the entire soil profile. Among these data, soil moisture storage in the 0-200 cm soil layer simulated by 94 GLDAS (Global Land Data Assimilation Systems) Noah (Rodell et al., 2004) has been most 95 extensively applied. However, soil thickness is not spatially uniform in reality, and the 200 cm depth fails to represent actual soil profile depth in many regions. As early as 2001, Rodell and Famiglietti 96 97 (2001) declared that a uniform soil depth of 200 cm would introduce significant uncertainties into 98 GRACE-derived GWSA estimation. They defined the remaining water storage in the unsaturated zone 99 below 200 cm as intermediate zone storage (IZS), a potentially critical but poorly understood 100 component of TWS. When IZS is not quantified, it is unrealistic to clearly determine to what extent the 101 separated GWSA variations are attributed to changes in actual groundwater level instead of changes in 102 deep-layer soil moisture storage (Rodell and Famiglietti, 2002). In regions where soil moisture acts as 103 the dominant component of TWS (Felfelani et al., 2017; Wang et al., 2018), the absence of deep-layer 104 soil moisture storage will inevitably diminish the accuracy of GWSA estimation. 105 The primary objective of this study is to develop an improved GRACE-derived GWSA dataset at 106 the global scale, namely igGWSA, by comprehensively considering diverse non-groundwater 107 components and particularly resolving the effects of deep-layer soil moisture storage. igGWSA is 108 expected to improve our understanding of the evolution of global and regional GWS, and to shed light 109 on the scientific management and sustainable utilization of groundwater resources under a changing 110 environment.

components to changes in GWS, which will consequently compromise the accuracy of GWSA

2. Datasets

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112	2.1. GRACE-based terrestrial water storage anomaly (TWSA) reconstruction data

113 In spite of the capability of providing global observations, the temporal gap existing between GRACE

and GRACE-FO is not conducive to the analysis of TWS evolution. To this end, Li et al. (2021)

115 reconstructed a long-term and gap-free TWSA dataset named GRID_CSR_GRACE_REC based on

116 RL06 GRACE Mascon solutions. This reconstruction showed high consistency with RL06 GRACE-FO

117 Mascon solutions and proved to be superior to previous TWSA datasets. Therefore,

118 GRID_CSR_GRACE_REC was adopted in this study to encompass the entire period from 2000 to

119 2019.

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2.2. Non-groundwater components data

121 **2.2.1. Glaciers**

- 122 Taking advantage of massive stereo images from the Advanced Spaceborne Thermal Estimation and
- 123 Reflection Radiometer (ASTER), Hugonnet et al. (2021) developed a global-scale glacier mass balance
- 124 dataset. Changes in glacier surface elevation, volume and mass were estimated at four levels of spatial
- 125 resolution, i.e., $0.5^{\circ} \times 0.5^{\circ}$, $1^{\circ} \times 1^{\circ}$, $2^{\circ} \times 2^{\circ}$, and $4^{\circ} \times 4^{\circ}$. Volume change data with the finest resolution
- 126 $(0.5^{\circ} \times 0.5^{\circ})$ were used in this study to obtain glacier water storage (Text S1).

127 **2.2.2. Permafrost**

- 128 Changes in permafrost water storage were indirectly estimated based on changes in active layer
- 129 thickness (ALT) in this study (Text S2), as suggested by Xiang et al. (2016) and Zou et al. (2022). ALT
- data were derived from Community Land Model version 5 (CLM5) developed by the National Center
- 131 for Atmospheric Research (NCAR).

132 **2.2.3. Snow**

- 133 Snow water equivalent simulations from seven reanalysis products were collected in this study,
- 134 including: (1) GLDAS Noah from NASA (Rodell et al., 2004); (2) GLDAS Variable Infiltration





135 Capacity (VIC) from NASA (Rodell et al., 2004); (3) GLDAS Catchment Land Surface Model (CLSM) 136 from NASA (Rodell et al., 2004); (4) Famine Early Warning Systems Network Land Data Assimilation 137 System (FLDAS) Noah from NASA (Mcnally et al., 2022); (5) Modern-Era Retrospective analysis for 138 Research and Applications version 2 (MERRA-2) from NASA (Gelaro et al., 2017); (6) The land 139 component dataset of the fifth generation of European ReAnalysis (ERA5-Land) from European Centre 140 for Medium-Range Weather Forecasts (ECMWF) (Munoz-Sabater et al., 2021); (7) Japanese 55-year 141 Reanalysis (JRA-55) from Japan Meteorological Agency (JMA) (Kobayashi et al., 2015). 142 2.2.4. Lakes and reservoirs 143 The global database of lake water storage (GLWS) developed by Yao et al. (2023) was used in this 144 study. To construct GLWS, 248,649 satellite images from Landsat were used to map time-varying water 145 areas (Yao et al., 2019). Then, elevation measurements from nine satellite altimeters, including CryoSat-2, ENVISAT, ICESat, ICESat-2, Jason 1-3, SARAL, and Sentinel 3, were used to estimate 146 147 water levels. Lastly, changes in lake volume were quantified by combining water areas with water 148 levels. GLWS depicts the variations in water storage of 1,972 large water bodies spanning 1992 to 2020, 149 accounting for 96% of the total global lake water storage and 83% of the total global reservoir water 150 storage, respectively. Data processing of GLWS is detailed in Text S3. 151 2.2.5. Surface runoff 152 The global runoff reanalysis reconstructed by Ghiggi et al. (2021), namely Global RUNoff 153 ENSEMBLE (G-RUN ENSEMBLE), was used in this study. G-RUN ENSEMBLE is produced based 154 on in situ river discharge measurements and machine learning. Benchmarked against other independent 155 observations, this reanalysis outperforms simulations from a set of global hydrological models. A total 156 of 21 atmospheric forcing datasets are involved to generate 525 ensemble members in G-RUN 157 ENSEMBLE, and the median of all these members was adopted in our study. 158 2.2.6. Plant canopy water

Plant canopy water simulations from four reanalysis products were collected in this study, including: (1)

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160 GLDAS Noah; (2) GLDAS VIC; (3) GLDAS CLSM; (4) ERA5-Land.

2.2.7. Profile soil moisture (PSM)

In most GRACE-derived GWSA studies, the depth of soil moisture profile is set fixed, say 200 cm and 289 cm in Noah model driven by GLDAS and CHTESSEL model driven by ERA5, respectively. In this study, PSM simulated by CLSM was utilized. Inspired by Famiglietti and Wood (1994), Koster et al. (2000) and Ducharne et al. (2000) proposed CLSM in 2000 by coupling a classic hydrological model, TOPMODEL (Beven and Kirkby, 1979), with the parameterization of surface energy and water fluxes from Mosaic LSM. Based on the concepts of TOPMODEL, the distribution of water table depth can be inferred from that of topographic index. Subsequently, the distribution of water table depth is applied to derive catchment deficit (CD), which is defined as the water amount required to saturate the entire catchment under the assumption that vertical moisture profile in the unsaturated zone arises from hydrostatic equilibrium. In addition, two variables that take into account non-equilibrium conditions are defined in CLSM, namely surface excess (SE) and root zone excess (RE). SE and RE quantify the deviations of surface soil moisture and root zone soil moisture, respectively, from the value implied by the equilibrium profile. Richards equation is used to solve the vertical water fluxes between CD, SE, and RE, which contribute to bringing the vertical moisture profile closer to the equilibrium profile (Gascoin et al., 2009). Despite the significant value of CLSM-simulated PSM, uncertainties inherent to single-source simulation may inevitably compromise the accuracy of GWSA estimation. Thus, machine learning was applied in this study to improve CLSM-simulated PSM, as will be detailed in Sect. 3.2.

2.3. Predictor variables for PSM

Root zone soil moisture (RZSM), meteorological variables, and vegetation index were selected as predictor variables for PSM. As a function of vegetation type, root zone depth is characterized by spatial heterogeneity and is inherently challenging to quantify globally. In this study, soil water content within the uppermost 100 cm soil layer was defined as RZSM as suggested by Xu et al. (2021) and Heyvaert et al. (2023). RZSM simulations from five reanalysis products were collected, including: (1) GLDAS Noah; (2) GLDAS CLSM; (3) FLDAS Noah; (4) MERRA-2; (5) ERA5-Land. Data

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interpolation.





processing of RZSM is detailed in Text S4. With regard to meteorological variables, air temperature and precipitation from one of the most widely used climate dataset, CRU TS (Climatic Research Unit gridded Time Series) v4.08 (Harris et al., 2020), was adopted. Besides, the normalized difference vegetation index (NDVI) provided by Global Inventory Monitoring and Modeling System (GIMMS) (Pinzon and Tucker, 2014) was also used for prediction of PSM. 2.4. In situ-observed and model-simulated groundwater data Jasechko et al. (2024) compiled in situ observations of groundwater level (GWL) from a total of 170,000 wells and 1,693 aquifer systems across more than 40 countries worldwide, with which they revealed widespread groundwater depletion in the 21st century. Due to the provisions of data sharing, only 59% of data used for analysis can be publicly accessed. The available data exhibit a pronounced spatial imbalance, with 97.7% of the monitoring wells located in the United States and the remaining 2.3% distributed across China, Canada, Europe, etc. In situ-observed GWL served as the benchmark for validating GWSA estimation in this study. In addition, a state-of-the-art hydrological model coupled with human activity modules, namely the WaterGAP Global Hydrological Model (WGHM), was employed to provide independent simulations of GWSA. WaterGAP (Water-Global Assessment and Prognosis) is developed by the University of Frankfurt to quantify water storage, water resources, and water use at the global scale. GWSA simulations from the most recent version, i.e., WaterGAP v2.2e (Schmied et al., 2024), were used in this study. Detailed information of data utilized in this study is listed in Table 1. Taking into account the spatiotemporal attributes of diverse datasets, this study was conducted over global land areas excluding Antarctica (60 °S-90 °N) at a 0.5° ×0.5° spatial resolution, spanning the period from January 2000 to

December 2019. Datasets with coarser resolutions were harmonized to $0.5^{\circ} \times 0.5^{\circ}$ by using bilinear





Table 1. Detailed descriptions of data utilized for generating igGWSA.

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Variable	Data source	Time span	Temporal	Spatial extent	Spatial resolution	Reference
			resolution			
TWS	GRID_CSR_GRACE_REC	1979–2020	monthly	No 06-So 09	0.5° ×0.5°	Li et al. (2021)
Glacier mass balance	ASTER-based	2000–2019	monthly	global	0.5° × 0.5°	Hugonnet et al. (2021)
Active layer thickness	CLM5	1850-present	monthly	global	$1.25^{\circ} \times 0.9375^{\circ}$	Lawrence et al. (2019)
Snow water	GLDAS Noah	2000-present	monthly	No 06-So 09	0.25 % 0.25 °	Rodell et al. (2004)
equivalent	GLDAS VIC	2000-present	monthly	N _o 06-S _o 09	1 % 1 °	Rodell et al. (2004)
	GLDAS CLSM	2000-present	monthly	N _o 06-S _o 09	1 % 1 °	Rodell et al. (2004)
	FLDAS Noah	1982-present	monthly	N _o 06-S _o 09	0.1 % 0.1 °	Mcnally et al. (2022)
	MERRA-2	1980-present	monthly	N _o 06–S _o 09	0.625 ~ 0.5 °	Gelaro et al. (2017)
	ERA5-Land	1950-present	monthly	global	0.1 % 0.1 °	Muñoz-Sabater et al. (2021)
	JRA-55	1958-present	monthly	global	0.5625×0.5625 °	Kobayashi et al. (2015)
Lakes and reservoirs	GLWS	1992–2020	near-monthly	global	individual lake	Yao et al. (2023)
Surface runoff	G-RUN ENSEMBLE	1902–2019	monthly	global	$0.5^{\circ} \times 0.5^{\circ}$	Ghiggi et al. (2021)
Plant canopy water	GLDAS Noah	2000-present	monthly	N _o 06–S _o 09	0.25 % 0.25 °	Rodell et al. (2004)
	GLDAS VIC	2000-present	monthly	N _o 06–S _o 09	1 % 1 °	Rodell et al. (2004)
	GLDAS CLSM	2000-present	monthly	N _o 06–S _o 09	1 % 1 °	Rodell et al. (2004)
	ERA5-Land	1950-present	monthly	global	0.1 % 0.1 °	Muñoz-Sabater et al. (2021)





Table 1 (continued). Detailed descriptions of data utilized for generating igGWSA.

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Variable	Data source	Time span	Temporal	Spatial extent	Spatial resolution	Reference
			resolution			
Profile soil moisture	GLDAS CLSM	2000-present	monthly	No 06-So 09	1 % 1 °	Rodell et al. (2004)
Root zone	GLDAS Noah	2000-present	monthly	No 06-So 09	0.25 % 0.25 °	Rodell et al. (2004)
soil moisture	GLDAS CLSM	2000-present	monthly	N _o 06–S _o 09	1 % 1 °	Rodell et al. (2004)
	FLDAS Noah	1982-present	monthly	N _o 06–S _o 09	0.1 % 0.1 °	Mcnally et al. (2022)
	MERRA-2	1980-present	monthly	N _o 06–S _o 09	0.625 × 0.5 °	Gelaro et al. (2017)
	ERA5-Land	1950-present	monthly	global	0.1 % 0.1 °	Muñoz-Sabater et al. (2021)
Precipitation	CRU TS v4.08	1901-present	monthly	N _o 06–S _o 09	0.5° × 0.5°	Harris et al. (2020)
Temperature	CRU TS v4.08	1901-present	monthly	N _o 06–S _o 09	0.5° × 0.5°	Harris et al. (2020)
NDVI	GIMMS	1982–2022	semi-monthly	global	$0.083^{\circ} \times 0.083^{\circ}$	Pinzon and Tucker (2014)
Groundwater level	in situ	well-dependent	yearly	global	individual well	Jasechko et al. (2024)
GWSA _{WGHM}	WaterGAP v2.2e	1901–2019	monthly	global	0.5° × 0.5°	Schmied et al. (2024)

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3.1. Integrating multi-source estimates via Bayesian three-cornered hat (BTCH)

BTCH proposed by He et al. (2020) is a data fusion method free of any a priori knowledge. By

216 coupling TCH technique with Bayesian probabilistic frameworks, BTCH is capable of reducing

uncertainties inherent to single-source dataset, and has been widely used to improve the estimation of

218 hydrological variables such as soil moisture (Shangguan et al., 2023) and terrestrial water storage

(Chen et al., 2024). In this study, BTCH was employed to generate ensemble simulations of snow water

equivalent, plant canopy water and RZSM (Fig. 1, Text S5).

3.2. Generating PSM data with lower uncertainties via machine learning

222 **3.2.1. Random forest (RF)**

223 RF is an ensemble machine learning technique that combines decision tree with bagging algorithm

224 (Breiman, 2001). In contrast to non-ensemble techniques, RF is characterized by stronger

225 generalization ability, higher robustness to noise, and lower susceptibility to overfitting. Moreover, RF

226 is more interpretable than other black-box machine learning methods owing to its capability to quantify

227 the relative importance of predictors. RF has been extensively applied in soil moisture prediction

228 (Wang et al., 2022; Li et al., 2022).

3.2.2. Modelling the relationship between PSM and covariates

230 RF was employed to establish relationship model between CLSM-simulated PSM and diverse

231 covariates including CLSM-simulated RZSM, air temperature, precipitation, and NDVI (Fig. 1). There

are two key hyperparameters in RF: the number of trees (ntree) and the number of variables randomly

sampled as candidates at each split (mtry). We adjusted ntree from 250 to 1000 in steps of 250, and

varied mtry from 1 to 4 (the total number of predictors) in steps of 1. All the remaining parameters

were retained at their default settings. The 16 combinations of ntree and mtry were tested one by one,

among which the one with the lowest prediction error was determined as the optimal parameter





237 combination. Based on the optimal hyper-parameters, prediction models for PSM were developed at 238 the pixel scale by randomly partitioning the datasets into training set and validation set at an 80%:20% ratio. The accuracy of RF model was evaluated using two metrics: R² (coefficient of determination) and 239 240 rRMSE (relative root mean square error) (Text S6). 241 To further quantify the spatial differences in the accuracy of RF models, performance evaluation 242 was also conducted at the climatic zone scale. Here, climate classification scheme based on aridity 243 index (AI), the ratio of annual precipitation to potential evapotranspiration (PET), was adopted as 244 suggested by the United Nations Environment Program (UNEP) (Middleton and Thomas, 1997). The 245 climatology (1991-2020) of AI was computed using precipitation and PET data provided by CRU TS 246 v4.08. Following the definition of UNEP, humid regions (AI≥0.65) and drylands (AI<0.65) were first 247 delineated with a threshold of 0.65. Whereafter, drylands were further classified into four subtypes: dry 248 sub-humid $(0.5 \le AI \le 0.65)$, semi-arid $(0.2 \le AI \le 0.5)$, arid $(0.05 \le AI \le 0.2)$, and hyper-arid 249 (AI<0.05). 250 3.2.3. Prediction of improved PSM and uncertainty analysis 251 Owing to the fact that PSM is inclusive of RZSM, this study assumed that RZSM served as a critical 252 predictor for PSM. Accordingly, the prediction accuracy of PSM was expected to be enhanced by 253 constraining the uncertainties in RZSM input. To this end, we integrated multi-source RZSM 254 simulations by using BTCH. Given the established optimal models, ensemble RZSM, air temperature, 255 precipitation, and NDVI were reintroduced as inputs into the models to derive improved prediction of 256 PSM that synthesized the advantages of multi-source soil moisture datasets (Fig. 1). 257 Quantitative analysis was imperative to demonstrate whether the uncertainties in the improved 258 prediction had been reduced relative to the original CLSM simulations. Typically, this can be achieved 259 by using in situ measurements as benchmarks. Nevertheless, unlike surface soil moisture or RZSM, in 260 situ-observed PSM is extremely scarce. In light of this, an alternative approach named the generalized 261 three-corner hat (GTCH) (Tavella and Premoli, 1994) was used for uncertainty analysis. Note that at 262 least three estimates are required to implement GTCH. Besides improved PSM and CLSM-simulated 263 PSM, we additionally derived GLDAS-Noah-based PSM, FLDAS-Noah-based PSM,

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264 ERA5-Land-based PSM, and MERRA-2-based PSM by replacing the ensemble RZSM with the 265 corresponding single-source RZSM as a model input. A dimensionless index, namely relative 266 uncertainty, was calculated by GTCH to evaluate the abovementioned six PSM estimations from the 267 perspective of uncertainties. 268 3.3. Estimation, validation and intercomparison methods of GWSA 269 3.3.1. Estimation of igGWSA and non-improved GWSA 270 Vertically, TWS comprises a variety of hydrological components such as glaciers, snow, soil moisture, 271 groundwater, etc. By subtracting diverse non-groundwater components, GWS can be isolated from 272 TWS (Fig. 1), as shown in Eq. (1). 273 $igGWSA = TWSA - GlacierWSA - PWSA - LRWSA - SRSA - PSMSA_{improved} - SWEA - PSMSA_{improved}$ 274 CWSA, (1) 275 where igGWSA stands for the improved estimation of groundwater storage anomaly; TWSA is 276 terrestrial water storage anomaly; GlacierWSA is glacier water storage anomaly; PWSA is permafrost water storage anomaly; LRWSA is lake and reservoir water storage anomaly; SRSA is 277 278 surface runoff storage anomaly; PSMSA_{improved} is the improved profile soil moisture storage 279 anomaly; SWEA is snow water equivalent anomaly; CWSA is canopy water storage anomaly. 280 To quantify the impacts of incomprehensive considerations of non-groundwater components, five 281 kinds of non-improved GWSA were further estimated as listed below. 282 (1) GWSA_{simplified}: Similar to most previous studies (Liu et al., 2023; Peng et al., 2021; Zhao et al., 2023), simplified GWSA was separated from TWSA by subtracting only soil moisture storage 283 284 in the 0-200 cm soil layer, snow water equivalent, and plant canopy water simulated by 285 GLDAS Noah. 286 (2) GWSA_{CLSM}: CLSM-simulated PSM instead of improved PSM was used to estimate GWSA,

(3) GWSA₂₈₉: Soil moisture storage in the 0-289 cm soil layer derived from ERA5-Land instead of

improved PSM was used to estimate GWSA, with all other non-groundwater components

with all other non-groundwater components identical to those for igGWSA.

calculated to facilitate the validation.





290 identical to those for igGWSA. 291 (4) GWSA₂₀₀: Soil moisture storage in the 0-200 cm soil layer derived from FLDAS Noah instead 292 of improved PSM was used to estimate GWSA, with all other non-groundwater components 293 identical to those for igGWSA. (5) GWSAignored: GlacierWSA was ignored when estimating GWSA, with all other 294 295 non-groundwater components identical to those for igGWSA. 296 3.3.2. Validation of igGWSA against in situ observations and model simulations 297 Focusing on the potential of igGWSA in detecting groundwater resources evolution and serving for 298 global water security, validation of igGWSA was performed in five globally recognized hotspots of 299 groundwater depletion, i.e., North China Plain, California Central Valley, High Plains of USA, Ganges-Brahmaputra River Basin, and the Middle East. 300 301 Among the five hotspots, high-density in situ observations of monitoring wells can be obtained from 302 Jasechko et al. (2024) in North China Plain, California Central Valley, and High Plains of USA. Given the intrinsic disparity in spatial scales between in situ monitoring (point-scale) and igGWSA (0.5° ×0.5 303 304 o grid cell), scale transformation was imperative before validation. Accordingly, point-scale data were 305 first converted into pixel-scale by averaging observations of wells located in the specific grid cell. Then in situ GWL and GWSA estimation at a $0.5^{\circ} \times 0.5^{\circ}$ resolution were upscaled to obtain basin-averaged 306 307 time series. Due to the fact that GWL and GWS are two fundamentally distinct hydrological variables, 308 error metrics such as RSME were unsuitable for validation. Instead, Pearson's correlation coefficient 309 (PCC) was employed to evaluate the consistency in their temporal evolution. 310 As for Ganges-Brahmaputra and the Middle East, in situ observations were currently unavailable. Alternatively, an advanced global hydrological model with consideration of effects of anthropogenic 311 312 activities (e.g., water withdrawal) on groundwater resources, i.e., WGHM, was introduced to provide 313 independent GWSA simulations. PCC between our igGWSA and WGHM-simulated GWSA was also





3.3.3. Intercomparison between igGWSA and non-improved GWSA

316 Similar to intercomparison between various PSM estimations, GTCH was applied to quantify the relative uncertainty of igGWSA as well as four kinds of non-improved GWSA estimations, i.e., 317 $GWSA_{simplified}, \ GWSA_{CLSM}, \ GWSA_{289}, \ and \ GWSA_{200}. \ GWSA_{ignored} \ was \ not \ involved \ in \ GTCH$ 318 319 evaluation given that glaciers constitute only a minor fraction of global land areas. 320 In addition to pixel-wise uncertainty analysis, intercomparison between igGWSA and non-improved 321 GWSA was further carried out under three kinds of distinctive geographical environments. To be 322 specific, the three environments refer to glacier-covered regions, giant lakes, and deep-soil areas, 323 corresponding to the absence of glaciers, lakes and reservoirs, and deep-layer soil moisture, 324 respectively, in most previous studies when estimating GWSA in these regions. For glacier-covered regions, a dataset of global glacier outlines named the Randolph Glacier 325 326 Inventory (RGI) was utilized. RGI 6.0 defines 19 first-order glacier regions: (1) Alaska; (2) Western Canada and USA; (3) Arctic Canada (North); (4) Arctic Canada (South); (5) Greenland Periphery; (6) 327 328 Iceland; (7) Svalbard and Jan Mayen; (8) Scandinavia; (9) Russian Arctic; (10) North Asia; (11) 329 Central Europe; (12) Caucasus and Middle East; (13) Central Asia; (14) South Asia (West); (15) South 330 Asia (East); (16) Low Latitudes; (17) Southern Andes; (18) New Zealand; (19) Antarctic and 331 Subantarctic. Region 19 was excluded from analysis. Intercomparison between igGWSA and 332 GWSA_{ignored} was conducted in glacier-covered regions. 333 For giant lakes, 13 lakes or lake clusters were involved: (1) Caspian Sea; (2) Great Lakes of North 334 America; (3) Victoria; (4) Tanganyika; (5) Baikal; (6) Great Bear; (7) Malawi; (8) Great Slave; (9) 335 Winnipeg; (10) Ladoga; (11) Balkhash; (12) Aral Sea; (13) Lakes of Tibetan Plateau. The outlines of 336 these lakes were derived from HydroLAKES dataset. Intercomparison between igGWSA and 337 GWSA_{simplified} was conducted in giant lakes. 338 For deep-soil areas, eight regions were selected as typical cases: (1) Mississippi River Basin; (2) 339 Volga River Basin; (3) Ob River Basin; (4) Loess Plateau; (5) Congo River Basin; (6) Songhua-Liaohe River Basin; (7) Pampas Steppe; (8) Ganges-Brahmaputra River Basin. These regions were primarily 340 341 determined based on soil depth information defined in GLDAS VIC model (Fig. S1) and encompassed 342 the major loess and chernozem zones worldwide. Intercomparison between igGWSA, GWSA289, and



343 GWSA₂₀₀ was conducted in deep-soil areas.

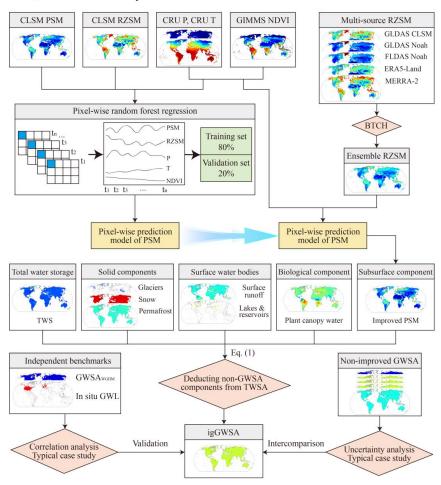


Figure 1. Flowchart of the generation process for igGWSA.

346 **4. Results**

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4.1. Performance evaluation of RF-based modelling of PSM

4.1.1. Evaluation at the pixel scale

- Pixel-wise RF models demonstrated exceptional accuracy in replicating CLSM-simulated PSM (Fig. 2).
- 350 During model training, 86.90% and 97.33% of global grid cells achieved R ²values exceeding 0.9 and
- 351 0.8, respectively, indicating strong explanatory power of the selected predictors for PSM. With regard



to error metric, rRMSE was contained below 1% and 2% for 93.47% and 99.87% of global grid cells, respectively. The accuracy of validation sets was relatively lower than that of training sets, with 67.14% and 83.07% of grid cells exhibited R ²values exceeding 0.9 and 0.8, respectively, and 76.96% and 97.43% of grid cells showed rRMSE less than 1% and 2%, respectively. Overall, the training and validation sets achieved average R ²values of 0.96 and 0.89, respectively, with average rRMSE values of 1.18% and 1.84%.

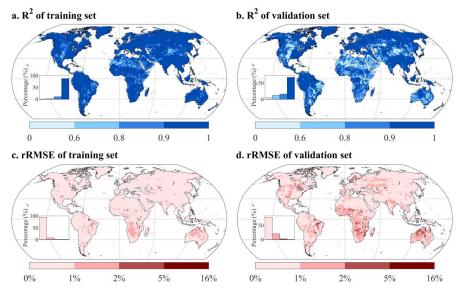


Figure 2. Pixel-scale performance of RF-based modelling of PSM.

4.1.2. Evaluation at the climatic zone scale

The accuracy of RF models was found to vary remarkably in different climatic zones. The models outperformed in humid regions compared to drylands, whether assessed through training/validation sets or evaluated by R 7 rRMSE (Fig. 3). For the training set, the average R 2 values were 0.98 and 0.93 for humid regions and drylands, respectively, and the average rRMSE values were 1.10% and 1.29%, respectively. Moreover, the predictive skill of RF models was observed to progressively decline with increasing aridity within drylands: dry sub-humid (R \geq 0.96), semi-arid (R \geq 0.94), arid (R \geq 0.92), and hyper-arid (R \geq 0.87).



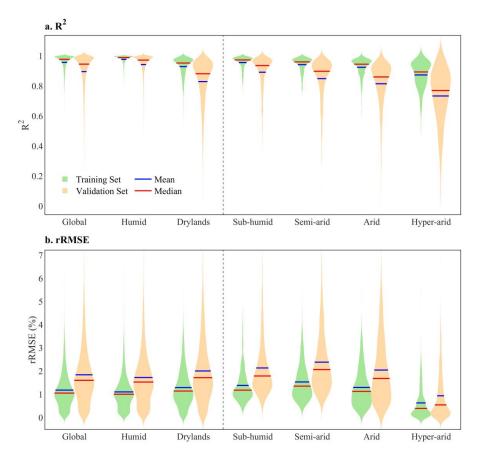


Figure 3. Climatic zone-scale performance of RF-based modelling of PSM.

4.1.3. Evaluation of interannual trends

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The aforementioned evaluations were achieved by randomly partitioning time series of the given pixel into training and validation sets without maintaining the original patterns. Given this, evaluation of interannual trends in PSM was carried out additionally. Results showed that trends in RF-predicted PSM were highly consistent with trends in CLSM-simulated PSM with R² exceeding 0.98 in all climatic zones (Fig. 4). RF models effectively reproduced the interannual variations in PSM, which was critical for the temporal patterns of the derived GWSA.



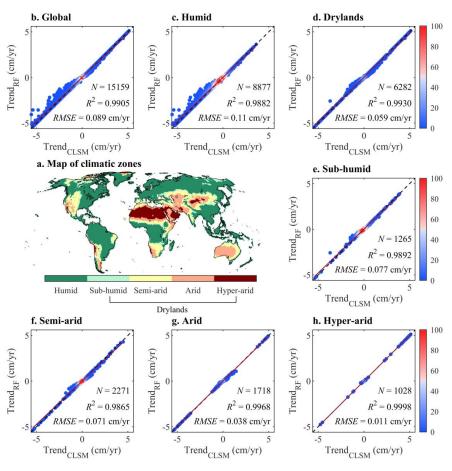


Figure 4. Comparison between trends in RF-predicted PSM and CLSM-simulated PSM.

4.2. Evaluation of improved estimation of PSM

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4.2.1. Intercomparison with fixed-depth soil moisture

Improved estimation of PSM (SMS_{profile}) was compared to soil moisture storage in 0–200 cm layer (SMS₂₀₀) and 0–289 cm layer (SMS₂₈₉) (Fig. 5). The multi-year (2000–2019) and global averages of SMS₂₀₀, SMS₂₈₉, and SMS_{profile} were 50.70 cm, 78.28 cm, and 106.98 cm, respectively. The spatial PCC between SMS₂₀₀ and SMS_{profile} was 0.55 (p<0.01), and that between SMS₂₈₉ and SMS_{profile} reached 0.74 (p<0.01). SMS₂₈₉ was more comparable to SMS_{profile} in both magnitude and spatial pattern, yet conspicuous deviations still existed. Therefore, fixed-depth soil moisture cannot adequately represent PSM, implying the considerable effects of deep-layer soil moisture.



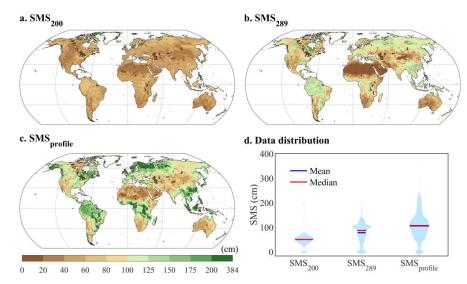


Figure 5. Intercomparison between SMS_{200} , SMS_{289} , and $SMS_{profile}$.

4.2.2. Intercomparison with single-source PSM estimations

Improved estimation of PSM was also compared to five kinds of single-source PSM estimations via GTCH (Fig. 6). The global-averaged relative uncertainty ranked as: CLSM-based PSM (0.057) > ERA5-Land-based PSM (0.048) > MERRA-2-based PSM (0.046) > GLDAS-Noah-based PSM (0.045) > FLDAS-Noah-based PSM (0.040) > ensemble-based PSM (0.019). CLSM-simulated PSM exhibited the highest uncertainty levels, whereas our improved PSM based on ensemble RZSM and RF modeling demonstrated the lowest relative uncertainty. Results confirmed that constraining the uncertainties of predictors can effectively improve the accuracy of PSM estimation.





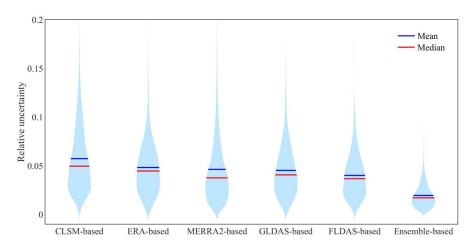


Figure 6. Relative uncertainty of ensemble-based PSM and single-source PSM.

4.3. Evaluation of igGWSA

4.3.1. Validation against in situ observations and model simulations

Well-monitored groundwater depth (GWD_{in situ}, negatively correlated with GWL) and WGHM-simulated GWSA (GWSA_{WGHM}) were applied as independent benchmarks to validate igGWSA in five typical hotspots (Fig. 7). PCCs between igGWSA and GWD_{in situ} reached $\neg 0.99$ (p < 0.01), $\neg 0.95$ (p < 0.01), and $\neg 0.96$ (p < 0.01) in North China Plain, Central Valley, and High Plains, respectively. Persistent declines in GWS were accompanied by distinct increases in GWD, both indicating substantial mass loss. For all the five hotspots, tremendous groundwater depletion revealed by igGWSA was highly consistent with GWSA_{WGHM} in spite of differences in declining rates, with PCCs ranging from 0.95 (p < 0.01) to 0.99 (p < 0.01). Validation results suggested that igGWSA was capable of detecting temporal evolution of groundwater resources. Unlike our comprehensive method, Jin and Feng (2013) obtained two GRACE-derived GWSA estimations based on GLDAS and WGHM by using simplified method and found that the amplitudes of GWSA_{WGHM} were much smaller than these two simplified estimations. In comparison, our igGWSA are in high agreement with GWSA_{WGHM} as demonstrated above, underscoring the importance of the full consideration of non-groundwater storage components.

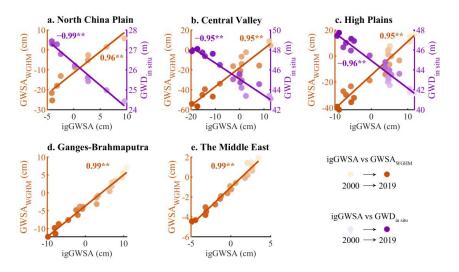


Figure 7. Validation of igGWSA against $GWD_{in\,situ}$ and $GWSA_{WGHM}$ in five typical hotspots of groundwater depletion. ** indicates significance at the 0.01 level.

4.3.2. Uncertainty analysis

Uncertainty analysis was further conducted for igGWSA and four kinds of non-improved estimations (Fig. 8). The global-averaged relative uncertainty ranked as: $GWSA_{simplified}$ (0.94) > $GWSA_{289}$ (0.74) > $GWSA_{CLSM}$ (0.67) > $GWSA_{200}$ (0.59) > igGWSA (0.56). The highest uncertainty was observed in $GWSA_{simplified}$, which was estimated by roughly deducting only fixed-depth soil moisture, snow, and plant canopy water from TWS like most previous studies. In contrast, our igGWSA that comprehensively took into account diverse non-groundwater components exhibited the lowest uncertainty. Note that $GWSA_{CLSM}$ relying on CLSM-simulated PSM showed higher uncertainty than igGWSA, highlighting the significance of improving GWSA estimation by optimizing PSM simulation.

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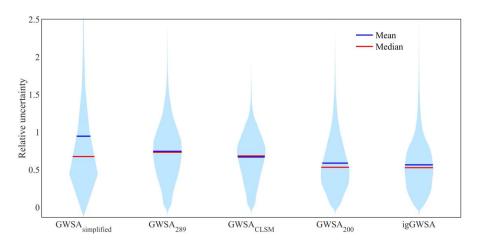


Figure 8. Relative uncertainty of igGWSA and non-improved estimations of GWSA.

4.4. Intercomparison between igGWSA and non-improved GWSA under distinctive geographical environments

4.4.1. Glacier-covered regions

The impacts of neglecting glacier water storage on the estimation of GWSA in glacier-covered regions manifested as three scenarios (Fig. 9, Table S2):

- (1) Misestimation of the sign of trends: In Region 1, 3, 4, 6, 7, 11, 13, 14, 15, and 17, GWS tended to increase significantly due to the replenishment from glacier meltwater. However, the potential increasing trends would be reversed when ignoring glacier as a non-groundwater component.
- (2) Overestimation of the decreasing trends: Both igGWSA and GWSA_{ignored} were observed to decrease, but the latter exhibited a more considerable declining rate on account of the additional contribution of changes in glacier. This pattern was found in Region 5, 9, and 12.
- (3) Underestimation of the increasing trends: Compared to igGWSA that increased at a remarkable rate, the increasing trend of $GWSA_{ignored}$ was greatly offset by glacier melting. This pattern was represented by Region 2, 8, 10, 16, and 18.

Regarding to the global glaciated areas, igGWSA and GWSA_{ignored} declined at rates of -0.19 cm/yr (p<0.01) and -4.03 cm/yr (p<0.01), respectively. However, the enormous mass loss signal was primarily attributed to glacier melting (-3.85 cm/yr, p<0.01) rather than groundwater depletion itself.



- 447 Therefore, absence of glaciers would inevitably result in inaccurate estimation of GWSA and
- 448 misunderstandings of GWS evolution in glacier-covered regions.

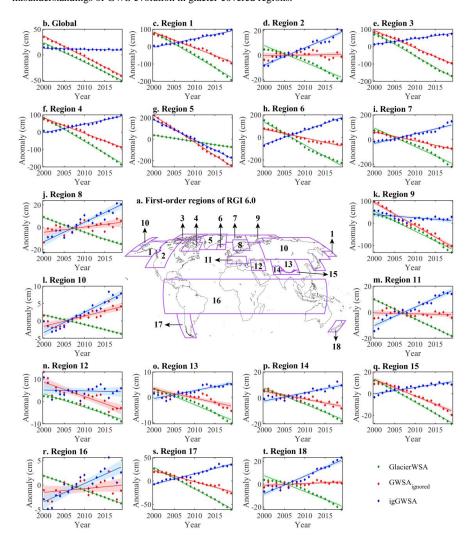


Figure 9. Intercomparison between igGWSA and GWSA $_{\rm ignored}$ in glacier-covered regions.

4.4.2. Giant lakes

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Among the 13 giant lakes, Tanganyika, Great Bear, Great Slave, Winnipeg, and Ladoga exhibited insignificant ($p \ge 0.05$) fluctuations in water storage. For the remaining eight lakes where dramatic storage variations have been detected, GWSA_{simplified} can lead to two kinds of diametrically opposed





455	misinterpretations (Fig. 10, Table S3).
456	(1) For shrinking lakes including Caspian Sea, Baikal, Malawi, and Aral Sea, increasing signals of
457	GWS were overshadowed by the pronounced declining signals of lake water storage, thus
458	indicating unrealistic risks of groundwater depletion.
459	(2) For expanded lakes including Great Lakes of NA, Victoria, Balkhash, and Lakes of Tibetan
460	Plateau, decreasing trends in GWS became unrecognizable due to the marked increasing trends
461	in lake water storage, consequently generating spurious positive signals of groundwater surplus.
462	This is what was exactly presented in Jin and Feng (2013).
463	For all the 1,972 large lakes and reservoirs worldwide, igGWSA and GWSA simplified showed a
464	decreasing trend of -0.19 cm/yr (p <0.01) and -0.35 cm/yr (p <0.01), respectively. GWSA _{simplified}
465	interpreted mass loss of surface water bodies (-0.11 cm/yr, $p>0.05$) as part of changes in GWS, which
466	significantly exaggerated groundwater depletion at the global scale

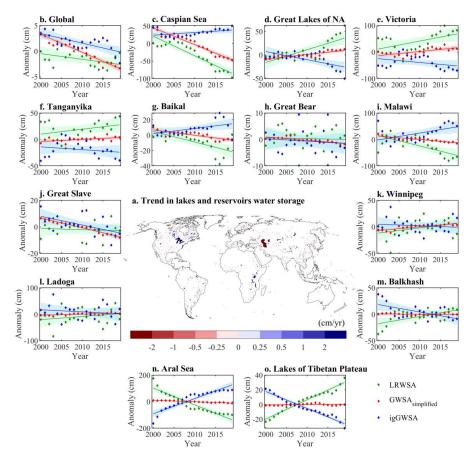


Figure 10. Intercomparison between ig GWSA and GWSA $_{\mbox{\footnotesize simplified}}$ in giant lakes.

4.4.3. Deep-soil areas

Non-improved GWSA based on fixed-depth SM (GWSA₂₀₀, GWSA₂₈₉) demonstrated consistent sign of interannual trends with igGWSA in only four of the eight deep-soil regions, i.e., Mississippi, Volga, Loess Plateau, and Ganges-Brahmaputra (Fig. 11, Table S4). GWSA₂₀₀ showed an opposite trend to igGWSA in Ob and Congo, and negative correlation was found between GWSA₂₈₉ and igGWSA in Songhua-Liaohe and Pampas. Beyond the sign, the magnitude of trends in GWSA₂₀₀, GWSA₂₈₉, and igGWSA also varied considerably. For instance, igGWSA exhibited insignificant fluctuations with absolute rates not exceeding 0.1 cm/yr in Ob, Congo, Songhua-Liaohe and Pampas. However, GWSA₂₈₉ increased significantly with rates ranging from 0.22 cm/yr to 0.69 cm/yr in these regions. Results underscored the limitations of fixed-depth SM data and the necessity of involving deep-layer

soil moisture as a non-groundwater component.

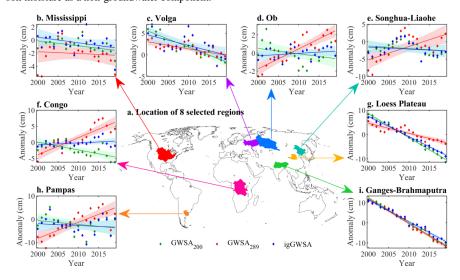


Figure 11. Intercomparison between $GWSA_{200}$, $GWSA_{289}$, and igGWSA in deep-soil areas.

5. Discussions

5.1. Influence factors of PSM modelling

In the RF-based modelling of CLSM-simulated PSM, CLSM-simulated RZSM achieved the highest importance among the four predictors across 97.17% of global grid cells (Fig. 12), implying the feasibility of improving PSM simulations by optimizing RZSM. Despite this, CLSM-simulated RZSM outperformed other RZSM products only in 16.10% of global grid cells (Fig. S2). The optimal RZSM product was characterized by strong spatial heterogeneity without any dominant patterns, which underscored the significance of integrating multi-source RZSM simulations for PSM prediction. Furthermore, the relative importance of RZSM varied with climate conditions. Specifically, it was more important in humid regions than in drylands as illustrated by scaled importance (Fig. S3). This implied the weaker correlation between RZSM and PSM in drylands, which explained the lower R2 of RF models in drylands mentioned in Sect. 4.1.2, given that RZSM was the foremost predictor of PSM. We attributed the differences across climatic zones to the higher susceptibility to decoupling of RZSM and PSM in drylands, which was consistent to Carranza et al. (2018) who identified decoupling of





surface and subsurface SM under arid conditions with in situ data.

For the remaining 2.83% of global grid cells, NDVI emerged as the dominant predictor variable for PSM modelling in most regions, accounting for 2.08% of global grid cells in total. Specifically, NDVI exhibited predominant impacts on PSM dynamics in the band between the Sahara Desert and the Congo Basin, the east coast of Africa, eastern South America, and northern Australia (Fig. 12). Interestingly, this spatial pattern closely aligned with the global distribution of deep-rooted regions predicted by Schenk and Jackson (2005) via climate-based model, highlighting the critical role of vegetation activity in regulating regional water storage variability. To further investigate the relationship between vegetation and water storage, the spatiotemporal variations of the sole vegetation-associated TWS component, i.e., canopy water storage (CWS), were analyzed (Fig. 84). However, the spatial pattern of CWS failed to match that of the variable importance of NDVI. The reason may be that CWS cannot adequately represent vegetation water storage, which was not quantified in this study due to its markedly smaller magnitude of variation compared to other components at the global scale (Rodell et al., 2005). Building on these findings, we suggest that vegetation water storage should be underscored in the hotspots of vegetation-PSM interactions to enhance the understanding of regional water storage evolution in future studies.

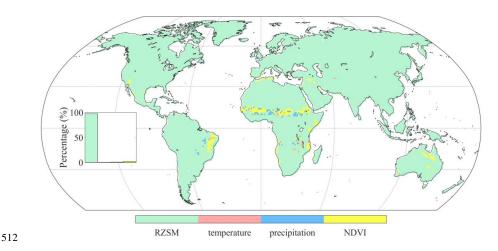


Figure 12. Map of dominant predictor variable for PSM modelling.

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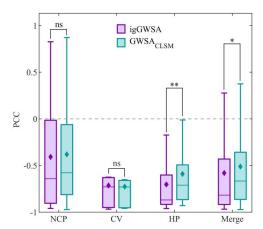
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5.2. The gains to GWSA estimation from improved PSM

As demonstrated in Sect. 4.3.2, igGWSA based on improved PSM achieved lower uncertainty compared to GWSA_{CLSM} based on CLSM-simulated PSM. To substantiate the gains from improved PSM to GWSA estimation, igGWSA and GWSA_{CLSM} were further compared using GWD_{in situ} as benchmarks. At the pixel scale, igGWSA showed average PCCs of -0.41, -0.71, -0.70, and -0.58 with GWD_{in} situ in North China Plain (NCP), Central Valley (CV), High Plains (HP), and the aggregation of these three hotspots, respectively. In contrast, average PCCs between GWSA_{CLSM} and GWD_{in situ} were -0.38, -0.73, -0.59, and -0.51 in these regions (Table 2). igGWSA achieved stronger correlations with GWD_{in situ} except in CV where only seven pixels were involved in analysis. Mann-Whitney U test was adopted to further identify the differences between igGWSA and $GWSA_{CLSM}$. The differences were not statistically significant in NCP and CV, while igGWSA was significantly superior to GWSA $_{\text{CLSM}}$ in HP and the aggregation (Fig. 13). At the regional scale, igGWSA and GWSA_{CLSM} exhibited comparable correlations with GWD_{in situ} in NCP and CV, with difference in PCCs not exceeding 0.02. As for HP, igGWSA was relatively more notably correlated with GWD_{in situ} than GWSA_{CLSM} (-0.96 vs -0.90) (Table 2). In conclusion, improving PSM via machining learning was of great significance for generating GWSA estimation with higher accuracy and lower uncertainty.



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Figure 13. Difference in PCC between igGWSA and $GWD_{in\ situ}$ versus $GWSA_{CLSM}$ and $GWD_{in\ situ}$ **





indicates significance at the 0.01 level; * indicates significance at the 0.05 level; ns indicates not significant (p > 0.05).

Table 2. Correlations of igGWSA and GWSA_{CLSM} with GWD_{in situ} at the pixel scale and the regional scale.

Danian	Pixel_N	Pixel scale		Regional scale	
Region		igGWSA	$GWSA_{CLSM}$	igGWSA	GWSA _{CLSM}
NCP	48	-0.41	-0.38	-0.99**	-0.98**
CV	7	-0.71	-0.73	-0.95**	-0.97**
HP	61	-0.70	-0.59	-0.96**	-0.90**
Merge	116	-0.58	-0.51	/	/

Note: Pixel_N indicates the number of pixels at a $0.5^{\circ} \times 0.5^{\circ}$ resolution in the specific region; ** indicates significance at the 0.01 level; Values for pixel scale indicates the average of PCCs for all pixels.

5.3. Uncertainties and limitations

Although GRACE provides an innovative perspective for monitoring GWS, it is essentially an indirect estimation methodology. Uncertainties inherent in TWSA data and non-groundwater components data will ultimately propagate into GRACE-derived GWSA. Therefore, validation of igGWSA against in situ measurements is imperative. However, existing as a conceptual derivative of TWSA, GWSA lacks ground truth. Given that, GWL data collected from monitoring wells can serve as substitute benchmarks for validating GWSA. It should be noted that GWL is closely linked to but is not directly comparable to GWSA. Accordingly, only correlation metric was employed for validation without error quantification in this study. Moreover, as mentioned in Sect. 1, the scarcity of globally accessible groundwater monitoring data renders large-scale validation of GWSA infeasible. To address this, local-scale validation was alternatively conducted focusing on several hotspots of groundwater depletion in this study based on available in situ observations and model simulations accounting for human water use. We would greatly appreciate if researchers worldwide could carry out supplementary validation of igGWSA using locally available in situ data.

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6. Data availability

- 556 Datasets used to develop igGWSA are publicly available and have been stated in the Datasets section.
- 557 Our igGWSA dataset is archived on Zenodo and can be freely downloaded at
- 558 https://doi.org/10.5281/zenodo.16871689 (Wang et al., 2025).

7. Conclusions

this study. To this end, we first generated improved estimation of PSM based on RF algorithm and

An improved GRACE-derived GWSA dataset over global land, namely igGWSA, was developed in

- $562 \qquad \text{multi-source RZSM simulations. Then diverse non-groundwater components were subtracted from} \\$
- 563 TWSA to obtain igGWSA. Finally, validation of igGWSA against in situ observations and model
- simulations and intercomparison between igGWSA and non-improved GWSA were conducted. The
- key conclusions can be summarized as follows:
- 566 (1) RF-based modeling of PSM exhibited superior performance at the global scale, with average R²
- and rRMSE reaching 0.96 and 1.18%, respectively. RF models outperformed in humid regions
- over drylands Among the predictors, RZSM showed the highest explanatory power for PSM
- variations, implying the feasibility of improving PSM by optimizing RZSM. The improved
- 570 PSM estimation integrating multi-source RZSM exhibited the lowest relative uncertainty
- 571 compared to estimations based on single-source RZSM.
- 572 (2) igGWSA was highly consistent with in situ-observed GWD and WGHM-simulated GWSA in
- five typical hotspots of groundwater depletion worldwide, i.e., North China Plain, California
- Central Valley, High Plains of USA, Ganges-Brahmaputra, and the Middle East, with |PCC|
- 575 ranging from 0.89 to 0.99. In addition, igGWSA exhibited the lowest relative uncertainty
- 576 compared to four kinds of non-improved GWSA estimations, including GWSA_{CLSM} that relied
- on CLSM-simulated PSM. Furthermore, igGWSA also achieved significantly stronger
- 578 correlations with in situ observations than GWSA_{CLSM}, underscoring the gains from improved
- 579 PSM to GWSA estimation.
- 580 (3) igGWSA and non-improved GWSA estimations showed remarkable discrepancies in





581 glacier-covered regions, giant lakes, and deep-soil areas. Specifically, neglecting glacier as a 582 non-groundwater component would erroneously attribute mass loss induced by glacier melting 583 to groundwater depletion. Similarly, simplified estimation without considering lakes and 584 reservoirs would confound the signals of lake shrinkage or expansion with changes in GWS. 585 Besides, GWSA estimations based on fixed-depth SM would fail to satisfactorily replicate the 586 sign and the magnitude of trends in igGWSA due to the absence of deep-layer soil moisture 587 storage. 588 Author contributions. ZW: Data curation, methodology, software, conceptualization, writing-original 589 590 draft, writing - review & editing. SL: Conceptualization, supervision, writing - review & editing, project administration, funding acquisition. XM: Supervision, writing - review & editing, project 591 592 administration, funding acquisition. 593 594 Competing interests. The contact author has declared that none of the authors has any competing 595 interests. 596 597 Acknowledgements. The authors would like to thank the institutions and scientists who contributed 598 invaluable data to the generation of our igGWSA dataset. 599 Financial support. This work was supported by National Key Research and Development Program of 600 601 China (Grant No. 2022YFF0801804), China National Natural Science Foundation Projects (Grant Nos. 12441511 and 12441501) and the Third Xinjiang Scientific Expedition Program (Grant No. 602 603 2021xjkk0803). 604 605 References Adams, K. H., Reager, J. T., Rosen, P., Wiese, D. N., Farr, T. G., Rao, S., Haines, B. J., Argus, D. F., 606 607 Liu, Z., Smith, R., Famiglietti, J. S., and Rodell, M.: Remote sensing of groundwater: current 608 capabilities and future directions, Water Resour. Res., 58, e2022WR032219, 609 https://doi.org/10.1029/2022wr032219, 2022. 610 Berghuijs, W. R., Luijendijk, E., Moeck, C., van der Velde, Y., and Allen, S. T.: Global recharge data set





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