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Key Points:

- A mascon-based GRACE terrestrial water storage product is assimilated into the Catchment model at the global scale
- GRACE data assimilation improved RMSE and correlation of simulated groundwater storage with in situ data at point and regional scales
- Uncertainty in model estimated water storage is strongly related to interannual variability of precipitation

Supporting Information:

- Supporting Information S1

Correspondence to:

B. Li,
bailing.li@nasa.gov

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Global GRACE Data Assimilation for Groundwater and Drought Monitoring: Advances and Challenges

Bailing Li^{1,2} , Matthew Rodell² , Sujay Kumar² , Hiroko Kato Beaudoin^{1,2} , Augusto Getirana^{1,2} , Benjamin F. Zaitchik³ , Luis Gustavo de Goncalves⁴, Camila Cossetin⁵, Soumendra Bhanja⁶ , Abhijit Mukherjee⁷ , Siyuan Tian^{8,9} , Natthachet Tangdamrongsab^{1,2} , Di Long¹⁰ , Jamiat Nanteza¹¹ , Jejung Lee¹² , Frederick Policelli², Ibrahim B. Goni¹³, Djoret Daira¹⁴, Mohammed Bila¹⁴, Gabriëlle de Lannoy¹⁵, David Mocko¹⁶, Susan C. Steele-Dunne¹⁷ , Himanshu Save¹⁸ , and Srinivas Bettadpur¹⁸ 

¹ESSIC, University of Maryland, College Park, MD, USA, ²Hydrological Sciences Laboratory, NASA Goddard Space Flight Center, Greenbelt, MD, USA, ³Department of Earth and Planetary Sciences, The Johns Hopkins University, Baltimore, MD, USA, ⁴Center for Weather Forecast and Climate Studies, National Institute for Space Research, São Paulo, Brazil, ⁵Climatempo, São José dos Campos, São Paulo, Brazil, ⁶Faculty of Science and Technology, Athabasca University, Athabasca, Alberta, Canada, ⁷Department of Geology and Geophysics, Indian Institute of Technology Kharagpur, Kharagpur, India, ⁸Research School of Earth Sciences, Australian National University, Canberra, ACT, Australia, ⁹Fenner School of Environment and Society, Australian National University, Canberra, ACT, Australia, ¹⁰Department of Hydraulic Engineering, Tsinghua University, Beijing, China, ¹¹Department of Geography, Geo-Informatics and Climatic Sciences, Makerere University, Kampala, Uganda, ¹²Department of Geosciences, University of Missouri, Kansas City, MO, USA, ¹³Department of Geology, University of Maiduguri, Borno State, Nigeria, ¹⁴Lake Chad Basin Commission, N'Djamena, Chad, ¹⁵Department of Earth and Environmental Sciences, Catholic University Leuven, Leuven, Belgium, ¹⁶Science Applications International Corporation, Reston, VA, USA, ¹⁷Department of Water Management, Civil Engineering and Geosciences, Delft University of Technology, Delft, The Netherlands, ¹⁸Center for Space Research, The University of Texas at Austin, Austin, TX, USA

Abstract The scarcity of groundwater storage change data at the global scale hinders our ability to monitor groundwater resources effectively. In this study, we assimilate a state-of-the-art terrestrial water storage product derived from Gravity Recovery and Climate Experiment (GRACE) satellite observations into NASA's Catchment land surface model (CLSM) at the global scale, with the goal of generating groundwater storage time series that are useful for drought monitoring and other applications. Evaluation using in situ data from nearly 4,000 wells shows that GRACE data assimilation improves the simulation of groundwater, with estimation errors reduced by 36% and 10% and correlation improved by 16% and 22% at the regional and point scales, respectively. The biggest improvements are observed in regions with large interannual variability in precipitation, where simulated groundwater responds too strongly to changes in atmospheric forcing. The positive impacts of GRACE data assimilation are further demonstrated using observed low-flow data. CLSM and GRACE data assimilation performance is also examined across different permeability categories. The evaluation reveals that GRACE data assimilation fails to compensate for the lack of a groundwater withdrawal scheme in CLSM when it comes to simulating realistic groundwater variations in regions with intensive groundwater abstraction. CLSM-simulated groundwater correlates strongly with 12-month precipitation anomalies in low-latitude and midlatitude areas. A groundwater drought indicator based on GRACE data assimilation generally agrees with other regional-scale drought indicators, with discrepancies mainly in their estimated drought severity.

1. Introduction

Groundwater, which accounts for 98% of the Earth's liquid freshwater, is one of the most important natural resources for the global community. More than 2 billion people rely exclusively on groundwater for drinking water, and 43% of irrigation water is supplied by aquifers (UNESCO, <https://en.unesco.org/themes/water-security/hydrology/groundwater>). Groundwater also plays a unique role in ecosystems, especially in semiarid regions and wetlands where rivers/lakes are sustained by groundwater discharge. Groundwater depletion commonly leads to reduced runoff (Hughes et al., 2012), disappearing riparian vegetation and

forests (Cunningham et al., 2011; Kath et al., 2014), and changes in other habitats (Stromberg et al., 1992). Understanding and accurately monitoring groundwater storage worldwide is essential for protecting this precious resource, for mitigating drought impacts, and for developing sustainable groundwater use strategies (Famiglietti, 2014).

In situ groundwater measurements are rarely available due to the cost associated with drilling and maintaining monitoring wells. Perhaps more importantly, where groundwater measurements are made, they frequently are not digitized and centralized, or they are withheld from the public due to political considerations (Rodell et al., 2009). In addition, observation wells are often limited in spatial coverage and may have discontinuous and/or short records, making them unsuitable for drought monitoring. Finally, confined and semiconfined aquifer data can be difficult to interpret for the purposes of groundwater storage accounting and drought monitoring.

Land surface models (LSMs) have been increasingly used to estimate groundwater storage changes, to examine the impact of climate variations and anthropogenic effects on groundwater (Crosbie et al., 2013; Pokhrel et al., 2012), and to monitor drought and wetness conditions (Houborg et al., 2012; Li et al., 2012). When forced by meteorological data, advanced LSMs can provide spatially and temporally continuous groundwater fields that reflect climate variations and are suitable for drought and water resource monitoring. LSMs constrained by both water and energy balances are capable of providing reasonably accurate evapotranspiration (ET) estimates (Jiménez et al., 2011; Mueller et al., 2011), which, along with high quality input precipitation and simulated drainage, is critical for simulating realistic groundwater storage changes (Eltahir & Yeh, 1999; Li et al., 2015). On the other hand, LSMs may contain highly simplified groundwater schemes (Koirala et al., 2014; Koster et al., 2000; Niu et al., 2007; Yeh & Eltahir, 2005a, 2005b) in comparison with dynamical groundwater flow models (e.g., de Graaf et al., 2015; Kollet & Maxwell, 2008). Oversimplification and lack of constraints on the temporal variability of groundwater cause inconsistency among groundwater change estimates from different LSMs, which may be larger than that of other hydrological variables such as soil moisture (Xia et al., 2017).

The Gravity and Recovery and Climate Experiment (GRACE) satellites mapped Earth's gravity field from April 2002 to July 2017. Temporal variations in gravity can be used to infer changes in total terrestrial water storage (TWS), which is the sum of soil moisture, groundwater, surface waters, snow and ice, canopy interception, and wet biomass. The GRACE observations, together with auxiliary information, led to significant scientific discoveries including detecting groundwater depletion caused by excessive groundwater withdrawals for irrigation in India, the U.S., China, the Middle East, and elsewhere (Famiglietti et al., 2011; Feng et al., 2013; Rodell et al., 2009; Rodell et al., 2018; Voss et al., 2013). GRACE data have also proved valuable in reducing the uncertainty associated with modeling anthropogenic effects on groundwater (e.g., Döll et al., 2014).

In parallel, techniques have been employed to assimilate GRACE data into LSMs in order to constrain model state variables while disaggregating and downscaling GRACE data. The latter is important because GRACE TWS data are typically monthly, with an effective spatial resolution around 150,000 km² at midlatitudes (Rowlands et al., 2005; Swenson et al., 2006). In earlier studies, GRACE TWS anomalies were aggregated over hydrological basins ranging from 100,000 to over a million square kilometers for assimilation into LSMs (Forman et al., 2012; Houborg et al., 2012; Li et al., 2012; Su et al., 2010; Zaitchik et al., 2008). The aggregation was consistent with the nature of spherical harmonic-based GRACE data products whose effective spatial resolution is coarse and which require filtering to reduce correlated errors (Landerer & Swenson, 2012). In recent years, new GRACE products based on regional mass concentration (mascon) functions have been developed with constraints applied during the inversion of satellite ranging observations (as opposed to after inversion) to better preserve GRACE signals (Rowlands et al., 2005; Save et al., 2012; Watkins et al., 2015). Direct assimilation of gridded GRACE data, which has been performed in recent studies (Tangdamrongsub et al., 2018; Eicker et al., 2014; Girotto et al., 2016, 2017; Kumar et al., 2016; Tangdamrongsub et al., 2015; Tian et al., 2017; van Dijk et al., 2014), not only preserves more of the observed information but also enables better alignment with existing infrastructures of land surface modeling, which are constructed on regular grids rather than irregular basins.

GRACE data provide unique information for drought monitoring not only because they detect water storage changes in the deeper subsurface but also because they are sensitive to water stresses throughout all seasons

(Li et al., 2012), which is important for continuous drought monitoring. Although GRACE TWS can be directly used for drought detection (e.g., Andersen et al., 2005; Chen et al., 2009; Getirana, 2016; Long et al., 2013; Rodell, 2012; Thomas et al., 2014; Zhao et al., 2017), data assimilation enables vertical disaggregation and spatial and temporal downscaling of GRACE data such that individual storage components such as groundwater can be monitored at scales finer than that of GRACE (around 150,000 km² at midlatitudes). In addition, a data-assimilating model forced by near-real-time meteorological data can generate up-to-date model estimates, which is critical for operational applications such as drought monitoring at a weekly basis (<https://droughtmonitor.unl.edu/>), and can fill observational gaps when GRACE data are not available (Houborg et al., 2012). This is especially useful during the transition period between GRACE and GRACE Follow On, which was launched in May 2018.

In this study, we employ an improved ensemble Kalman smoother implemented in the NASA Land Information System (LIS; Kumar et al., 2006) to assimilate a regularized, mascon-based GRACE TWS product (Save et al., 2016) into the Catchment land surface model (CLSM; Koster et al., 2000) for global-scale groundwater and drought monitoring. Previous studies on GRACE data assimilation into CLSM focused on the U.S. and Europe, where forcing data and models are relatively well constrained thanks to availability of observational data (Houborg et al., 2012; Kumar et al., 2016; Li et al., 2012; Zaitchik et al., 2008). Similar performance may not be expected in other parts of the world since the model was never calibrated and that errors in the atmospheric forcing fields vary depending on the availability of observations to constrain those fields (Sheffield et al., 2006). A global study is necessary for comprehensive and consistent (employing a common forcing data set) analysis of the impacts of GRACE data assimilation on modeled states and fluxes across different climate zones. Previous studies have shown that if a model overestimates the rate of TWS dry-down because it overestimates ET and/or runoff, increasing TWS through data assimilation will only exacerbate the high bias in those flux estimates, in addition to disturbing the water budget, the sum of ET, runoff, and TWS changes (Li et al., 2012). Because changes in the terrestrial water budget have been used to interpret changes in sea level and atmospheric moisture (Reager et al., 2016; Rodell et al., 2015; Wada et al., 2016), we analyze changes in the temporal variability of simulated TWS to deduce its impacts on ET, runoff, and the water balance.

Validation is crucial for demonstrating the usefulness of GRACE data and GRACE data assimilation for groundwater estimation, but it has been challenging due to dearth of in situ groundwater data. Therefore, we have compiled a significantly larger number of groundwater time series than did previous studies, sourced from nearly 4,000 wells across the world, to evaluate the benefits and limitations of GRACE data assimilation for simulating groundwater storage and to gain insight on how coarse-scale GRACE data can benefit fine-scale model estimates. Validation of simulated groundwater variations themselves is equally important for providing confidence in their application. Using this massive, multiyear validation data set, we analyze uncertainty in the simulated groundwater storage changes and its relationship with environmental factors such as climate. Such an analysis has been largely absent in previous global-scale groundwater studies (e.g., Döll et al., 2014; Gleeson et al., 2012; Sutanudjaja et al., 2018; Wada et al., 2012), with the exception of de Graaf et al. (2017), which used time series of groundwater data from the U.S. and the Rhine-Meuse basin to calibrate and evaluate a coupled dynamic groundwater model. Two innovations of this study are evaluation of simulated groundwater using (1) low-flow data from Global Runoff Data Center (GRDC, 2018) and (2) a global permeability data set (Gleeson et al., 2014) for comparisons across different hydrogeological settings.

Groundwater drought, defined as below-normal groundwater storage (Mishra & Singh, 2010), is mainly driven by long-term precipitation deficit (Bloomfield et al., 2019; Eltahir & Yeh, 1999; Li et al., 2015). Bloomfield et al. (2019) also showed that thick capillary fringes in the unsaturated zone may have played a role in the increase in groundwater drought frequency in a warming world. These studies suggest that both climate and hydrogeological conditions may influence the evolution of groundwater drought. We examine the temporal scales of groundwater drought using standard precipitation indices (SPIs) and their relationship with climate and model parameters. Finally, following the method of Houborg et al. (2012), we use the data assimilation output to produce a global groundwater drought indicator (GWI) and compare it with several regional-scale drought indicators. We describe CLSM in section 2, forcing and in situ data sets in section 3, and the ensemble Kalman smoother in section 4. Results on data assimilation and drought indices are presented in section 5, and the discussion and conclusions are provided in section 6.

2. Model

CLSM simulates subsurface water storage changes driven by land-atmosphere interactions (precipitation and ET) using three state variables: the surface excess and the root zone excess, which represent excessive soil moisture relative to the equilibrium state in the surface layer (0–2 cm below the surface), and the root zone (0–100 cm), respectively, and the catchment deficit, which represents the amount of water required to bring the profile to saturation (Koster et al., 2000). CLSM also simulates seasonal snowpack changes in three snow layers. CLSM does not model water table variations. Instead, groundwater storage is derived by subtracting the water stored in the root zone from that stored in the profile (which can be calculated from catchment deficit and other model parameters), whose capacity is determined by CLSM's bedrock depth parameter. The bedrock depth was uniformly increased by 2 m following Houborg et al. (2012), who showed that using the original bedrock depths, CLSM-simulated TWS often approached a lower limit in the southwestern U.S., such that it was unable to represent severe drought conditions. Other than that, the model was not modified or calibrated for this study. Since CLSM does not incorporate actual water table depths or aquifer thicknesses as input parameters, its simulated groundwater storage (not head as in a dynamic model) reflects the model parameterization (including bedrock depths). Thus, only the groundwater storage anomalies, not the total groundwater storage values or water table depths, are comparable with those of the in situ measurements.

CLSM does not simulate surface water (rivers and streams) or biomass water storage changes, which are small compared with soil moisture, groundwater, and snow water storage changes in much of the world (Rodell, Chao, et al., 2005; Rodell & Famiglietti, 2001). On the other hand, surface waters can dominate TWS variability in wet climates (Getirana et al., 2017). In those cases, our results should be interpreted such that surface water is a manifestation of groundwater where the water table intersects the land surface (Winter et al., 1998), and thus, surface water dynamics are reflected in the simulated groundwater. Further, CLSM does not simulate groundwater withdrawals or changes in icecaps and permanent snow cover, all of which are contained in the GRACE data. Given these limitations and assumptions, CLSM-based TWS is computed as the sum of water stored as canopy interception, snow water equivalent, root zone soil moisture, and unconfined and semiconfined groundwater.

In this study CLSM is run within LIS on a regular grid, as in Kumar et al. (2016), instead of on irregular hydrological basins as in earlier studies (Houborg et al., 2012; Li et al., 2012; Zaitchik et al., 2008). In each grid cell, subgrid-scale heterogeneity associated with topography is represented by three dynamically changing zones, representing the degree of saturation—saturated, transpiring, and wilting—within which different algorithms for ET and runoff are employed (Koster et al., 2000). CLSM-simulated ET has been compared with that from other global-scale LSMs and found to be similar in terms of capturing large-scale spatial patterns of annual ET and interannual variability (Jiménez et al., 2011; Mueller et al., 2011).

3. Data

3.1. Forcing Data Sets

The meteorological analysis fields from the operational European Center for Medium-range Weather Forecasts (ECMWF) Integrated Forecasting System (<https://www.ecmwf.int/en/forecasts/documentation-and-support/changes-ecmwf-model/ifs-documentation>) were used to force the model simulations from 2003 to present. These fields, which are provided on a 0.25° grid at a 3-hr interval, are generated by assimilating available atmospheric observations every 12 hr into a forecast model with surface meteorological fields such as precipitation and radiation diagnosed from the model output (Dee et al., 2011; Flemming et al., 2015).

For identifying groundwater drought, a climatology of groundwater storage reflecting the range of past variability is needed. This was generated by a CLSM simulation forced by the Princeton meteorological data set (Sheffield et al., 2006), which spans 1948–2012, because the ECMWF forcing data prior to 2003 were not available. The Princeton data set, which is provided on a 1° global grid (excluding the Antarctic) with a 3-hr time step, was derived by bias correcting the precipitation, solar radiation, and air temperature fields from the National Center for Environmental Prediction/National Center for Atmospheric Research reanalysis using in situ and satellite observations.

The climatology simulation run was begun by forcing CLSM with the Princeton forcing data from 1948 to 2012 with uniform initial conditions. Then the first 10 years of the simulation were discarded to remove the influence of model spin-up, and CLSM was restarted on 1 January 1948 using the mean states of 31 December of the remaining years (1959–2012) as initial conditions. Using the mean states as the initial conditions, as opposed to using those from a repeated model simulation based on forcing data from a single year, can reduce artifacts caused by extreme events such as drought during the spin-up period (Rodell, Houser, et al., 2005).

To ensure temporal consistency between the ECMWF-forced (2003 to present) and the Princeton-forced (1948–2012) simulations, the ECMWF forcing data were scaled so that the temporal mean of each field at each location matched that of the Princeton data during the overlapping period (2003–2012) following Li and Rodell (2014). An open loop CLSM simulation (i.e., without GRACE data assimilation) and a GRACE data assimilation (DA) simulation were performed using the scaled ECMWF forcing fields from March 2003 forward at 0.25° spatial resolution. The initial conditions for these two runs were taken from the output of the Princeton-forced climatology run.

3.2. GRACE Data

GRACE data used in this study were provided by the Center for Space Research (CSR) at the University of Texas and were derived using a regularized mass concentration (mascon) approach instead of the conventional spherical harmonic approach (Save et al., 2012; Save et al., 2016). The CSR mascon solution applies a time-variable regularization method to constrain the inversion of satellite ranging rates to gravity fields, thereby eliminating the need for postprocessing. Postprocessing of the GRACE data, for example, to remove correlated errors, has been shown to attenuate the retrieved signals (Landerer & Swenson, 2012; Save et al., 2012; Scanlon et al., 2016). The monthly CSR GRACE data are provided on a 0.5° global grid, although their effective spatial resolution is still around 150,000 km² due to the limitations of the measurement system. Still, it better preserves temporal and spatial details of GRACE signals compared with other products (Save et al., 2016).

Because GRACE derived TWS data are provided in the form of anomalies (departures from the long-term mean), we added the temporal mean of the model simulated TWS from the open loop run (averaged to each 0.5° GRACE grid) from 2003 to 2015 to the GRACE TWS anomalies (with their 2003–2015 mean removed) prior to data assimilation. The dynamic range of GRACE data was not scaled to that of the model as in Giroto et al. (2016, 2017). Further, the regularized mascon GRACE data set used here does not require the application of scale factors developed for the spherical harmonic based GRACE products (e.g., Landerer & Swenson, 2012).

3.3. In situ Groundwater

In situ groundwater data from the U.S., Brazil, India, China, Australia, Germany, France, the Netherlands, Nigeria, Chad, and Uganda (see the supporting information S1, for data sources and additional information) were obtained for evaluating the impact of GRACE data assimilation on simulated groundwater storage variations (Figure 1 and Table S1). Many of these wells have been used in previous studies for validating GRACE derived TWS and GRACE data assimilation (see the supporting information S1). In-depth analyses of well data in the U.S. and India including their relationship with climate can be found in Li et al. (2015) and Bhanja, Rodell, et al. (2017).

Following previous studies (Li et al., 2015; Rodell et al., 2007), we selected these wells based on three criteria: (1) the observed water levels exhibit seasonal variability throughout the data record, indicating that groundwater storage changes are controlled primarily by atmospheric processes (thus, wells in confined aquifers are excluded), which is consistent with what CLSM simulates; (2) the observations do not exhibit obvious signs of groundwater pumping or injection, which are not simulated by CLSM, such as sudden surges or declines in water levels; and (3) the observations span at least 5 years (2 years for Chad and Nigeria, Table S1) to ensure robust statistical analyses. Exceptions were made for wells in the North China Plain, where groundwater withdrawals for irrigation are extensive (Döll et al., 2014; Liu et al., 2011). Most of those time series show signs of abstractions such as sustained decline, though it is unclear if the declines were due to direct pumping from the well or represented ambient groundwater depletion. The affected wells were selected,

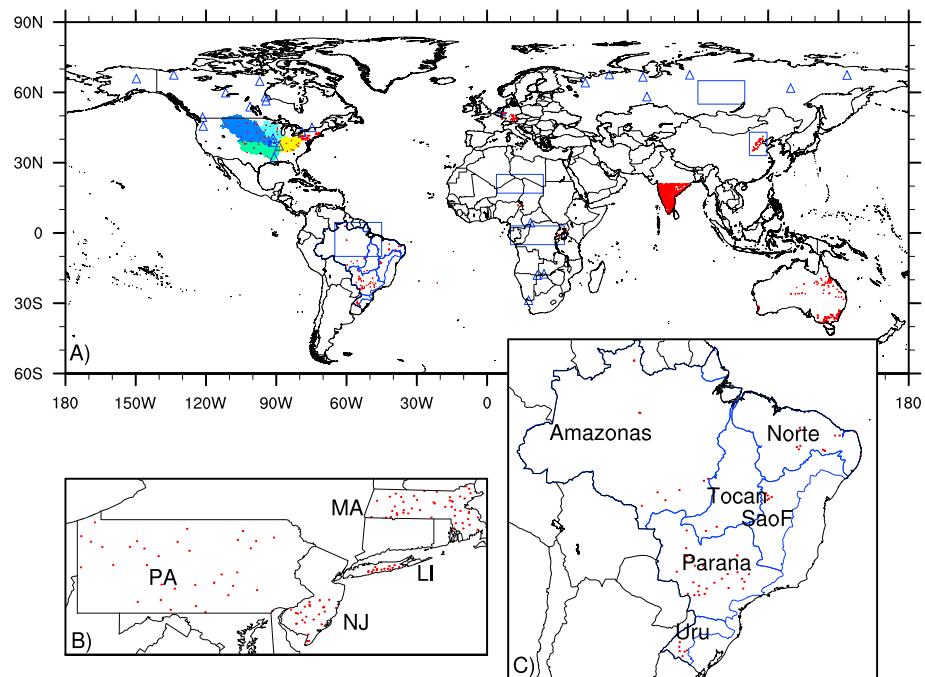


Figure 1. (a) Locations of groundwater observation wells (red dots) and GRDC streamflow stations (blue triangles) listed in Tables S1 and S3. Shaded areas represent the four subbasins of the Mississippi River: Missouri (dark blue), Upper Mississippi (light blue), Ohio-Tennessee (yellow), and Red River-Lower Mississippi (green). Blue rectangular regions are used to examine time series of TWS in Figure 2. (b) Well locations in the four northeastern U.S. regions. (c) Well locations in Brazil and their encompassing basins, Amazonas, Parana, Sao Francisco (SaoF), Uruguai (Uru), Tocantins (Tocant), and Atlantico Norte (Norte). Zoomed-in maps of well locations are provided in Figure S3.

as long as they also exhibited seasonal variability, to provide insight on the performance of GRACE data assimilation in areas where groundwater is being depleted (Döll et al., 2014).

To compare with CLSM-simulated groundwater storage (in mm), in situ data, which were provided either as depths to water or water table elevations, were converted to groundwater storage anomalies by first subtracting the long-term mean of each time series. For depth to water measurements, the additive inverse of the resulting anomalies was used to account for the fact that greater depth to water corresponds to less water storage. Finally, the anomalies were multiplied by location-specific estimates of specific yield to obtain groundwater storage anomalies as equivalent heights of water. Specific yield estimates were provided for wells in India and the North China Plain together with the groundwater observations. For wells located in the U.S., Brazil, Nigeria, and Chad, specific yield was estimated by reviewing published literature and using the available metadata (such as aquifer geological information), following the procedure outlined in Rodell et al. (2007) and Li and Rodell (2014). This set of specific yield values is provided in Table S2 (see the supporting information). Due to the lack of aquifer geological information for wells located in Uganda, Europe, and Australia, specific yield estimates were taken from the 0.5° global data set used by the PCRaster Global Water Balance (PCR-GLOBWB) model (Sutanudjaja et al., 2018). Note that CLSM simulates water storage changes directly and, thus, does not need specific yield as an input parameter.

3.4. GRDC Low-Flow Data

Groundwater contributes base flow that sustains rivers and streams in the dry season (Priest, 2004; Yang et al., 2017). Thus, changes in low flows reflect changing groundwater levels and can be used to evaluate interannual variability of simulated groundwater storage. Low-flow data are particularly useful given the inadequate spatial coverage of in situ groundwater measurements. Annual low-flow data were derived from monthly GRDC streamflow data (GRDC, 2018) at 27 stations (see Figure 1 and Table S3), which are located south of 70° N latitude in river basins with drainage areas $>150,000$ km². In addition, these stations have records that overlap the GRACE data assimilation period (2003–2017) for at least 10 years, resulting in at

least 10 annual low-flow observations at each station. Stations in managed basins such as the Colorado River basin or with zero low flow for consecutive years were excluded.

3.5. Permeability Data

Groundwater storage changes are influenced by hydrogeological properties such as permeability or hydraulic conductivity, in addition to climate. Evaluating the performance of CLSM and GRACE data assimilation across different hydrogeological settings may elucidate the environmental controls on groundwater storage changes. We use permeability, which reflects the ability of the subsurface medium to allow water flow through, estimated by Gleeson et al. (2014, Figure S1), to represent hydrogeological conditions. The data set was derived based on global lithology maps and calibrated permeability values for hydrolithologic units greater than 5 km and with upper boundaries less than 100 m deep. It consists of eight categories, ranging from unconsolidated sedimentary to volcanic rock (Figure S1).

3.6. Drought Indices

Groundwater drought in this study is defined as below-normal groundwater storage. The GWI is a ranking (percentile) of groundwater storage estimates from the GRACE data assimilation relative to the Princeton-based climatology (representing historical conditions). In addition to scaling the forcing fields as described in section 3.1, a set of scale factors, derived from the statistics of the GRACE data assimilation and Princeton-forced simulations for each calendar month, was applied to the modeled groundwater time series to ensure that groundwater drought was properly identified based on the long-term climatology at each location (Li & Rodell, 2014).

To evaluate the resulting GWI, we obtained regional drought products including the U.S. Drought Monitor (USDM, Svoboda et al., 2002), the Canadian Drought Monitor (Canadian DM, www.agr.gc.ca/atlas/cdm, excluding Nunavut), and the African Flood and Drought Monitor (African FDM, excluding the Sahara Desert; Sheffield et al., 2014). USDM and the Canadian DM are manually created by teams of authors based on their assessments (which may be subjective) of precipitation, temperature, soil moisture, and vegetation from in situ, remote sensing, and model sources, as well as information on local impacts from state climatologists and other sources. Similar to our GWI, the African FDM is based on percentiles of soil moisture simulated by the Variably Infiltration Community LSM. Because USDM and the Canadian DM provide five drought severity categories as opposed to percentiles, we used the following thresholds, as recommended by USDM, to convert GWI and African FDM percentiles to drought severity categories for comparison: D4 (exceptional drought): $< 2\%$, D3 (extreme drought): $2\text{--}5\%$, D2 (severe drought): $5\text{--}10\%$, D1 (moderate drought): $10\text{--}20\%$, D0 (abnormally dry): $20\text{--}30\%$.

4. Data Assimilation Method

Because the GRACE data are monthly averaged values, an ensemble Kalman smoother was used to assimilate GRACE-derived TWS into CLSM. For the given set of CLSM prognostics (including the three subsurface state variables, three state variables related to snow water equivalent, and one variable related to canopy interception), \mathbf{X}^f , the smoother assimilates GRACE observations into the modeled states through the update equation:

$$\mathbf{X}^a = \mathbf{X}^f + \mathbf{K}(\mathbf{Y}_o - \mathbf{Y}_M) \quad (1)$$

where \mathbf{X}^a represents the analysis of modeled states at the current time step; \mathbf{K} is the Kalman gain matrix, which depends on observation errors and model uncertainty determined from the ensemble; \mathbf{Y}_o represents observations, that is, GRACE-derived TWS; and \mathbf{Y}_M represents model prognostic TWS. Because GRACE TWS is an anomaly, \mathbf{Y}_o was created by adding the long-term temporal mean of modeled TWS to GRACE TWS as indicated earlier. Prognostic and analysis (\mathbf{X}^f and \mathbf{X}^a) are computed at the model's finer scale, that is, 0.25° and daily, while \mathbf{Y}_o and \mathbf{Y}_M are evaluated monthly at the coarser scale of GRACE data, 0.5° . This is an improvement over earlier studies in which the observations were either aggregated to large hydrological basins (Houborg et al., 2012; Li et al., 2012; Zaitchik et al., 2008) or interpolated to the finer-scale of the CLSM simulation (Kumar et al., 2016), in that it maintains the native resolution of the GRACE product. Note that the state and observation vectors, \mathbf{X} and \mathbf{Y} , as well as the Kalman gain matrix, \mathbf{K} , are time dependent but their time subscriptions have been omitted above for simplicity.

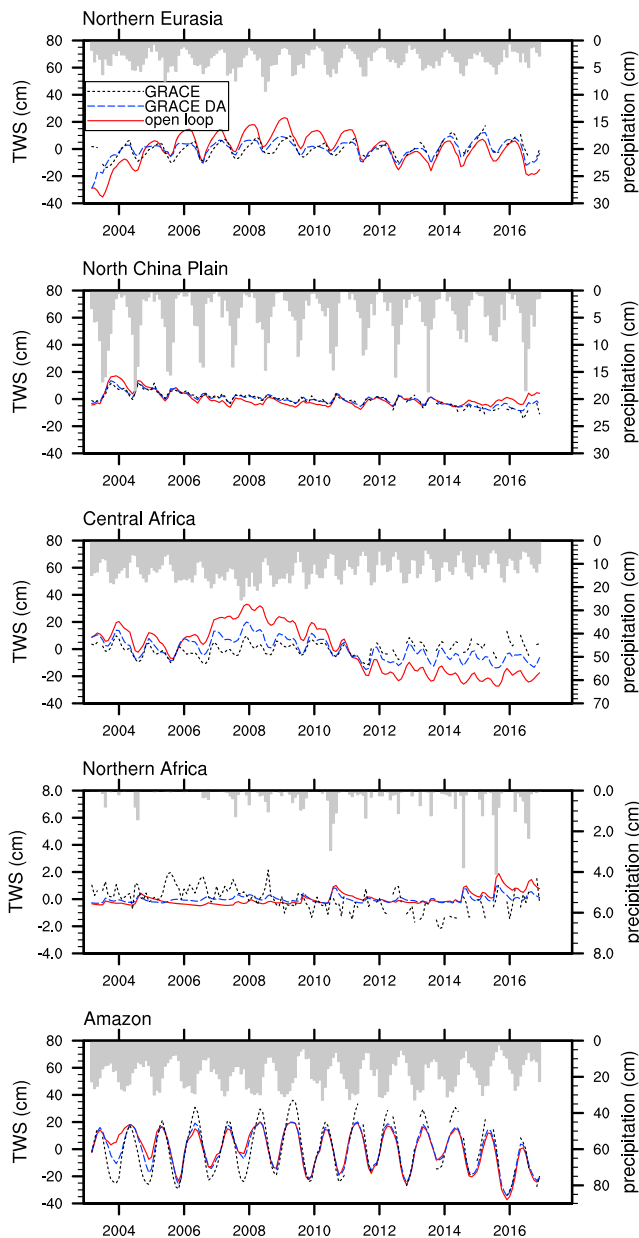


Figure 2. Monthly TWS anomalies (relative to the long-term temporal mean) from the open loop (OL), GRACE data assimilation (DA), and GRACE, with monthly ECMWF precipitation (shaded bars) for the rectangular regions shown in Figure 1. Note the different y axis scale in each panel for precipitation and a different scale for TWS in Northern Africa.

GRACE data assimilation failed to increase annual TWS maxima in most years to match the observations, which indicates that CLSM, even with the implemented 2-m increase in bedrock depth, does not possess enough water storage capacity to accommodate the strong TWS variability of the Amazon. Part of that issue is that CLSM does not represent surface water, which is a major component of TWS in the Amazon (Getirana et al., 2017).

In the northern Africa, OL TWS shows very little variability due to the scant precipitation. GRACE TWS shows stronger temporal variability including an overall decreasing trend, which may be associated with groundwater abstraction in the Sahara aquifers (Ahmed et al., 2014), an effect not simulated by CLSM. In addition, uncertainty in simulated TWS in this extremely dry climate is likely high due to the scarcity of

The smoother assimilates GRACE data in two iterations. During the first iteration, the ensemble members run forward from the first to the last day of each month to obtain monthly CLSM estimated TWS. In the second iteration, the updates or increments are calculated at the first day of the month and then divided by the number of days in that month and applied to daily states with fluxes adjusted accordingly (Zaitchik et al., 2008).

Following previous studies, random errors were added to three forcing fields (precipitation and short and long wave radiation), simulated surface excess and catchment deficit, and GRACE TWS, to represent uncertainty in the forcing data, model, and observations. All perturbation parameters and schemes (additive or multiplicative) are the same as in Reichle et al. (2007), Zaitchik et al. (2008), and Li et al. (2012), except a 0.3 multiplicative precipitation error and a 10-mm GRACE error were used in this study. The spatial correlation scale is 2° for both the observation and forecast error perturbations.

5. Results

5.1. Terrestrial Water Storage

Figure 2 shows spatially averaged monthly TWS anomalies (relative to temporal mean) from the open loop (OL, model simulation only), GRACE data assimilation (DA), and GRACE for the selected regions shown in Figure 1 (blue rectangles), along with monthly precipitation. In general, TWS shows strong seasonality, slightly lagging the seasonal cycle of precipitation. Seasonality of GRACE TWS is also strongly influenced by other climate conditions such as radiation and temperature (Humphrey et al., 2016). This is why, in the Northern Africa, where precipitation is less seasonal, TWS has a clear seasonal cycle. TWS also exhibits strong interannual variability in response to the interannual variability of precipitation. For instance, the apparent decreasing trend of TWS in the central Africa during 2008–2012 and the increasing trend in the northern Eurasia during 2003–2005 were associated with changing annual precipitation.

CLSM (OL) generally captured the multiscale TWS temporal variability seen in the GRACE data but in three of five regions simulated TWS responded more strongly to changes in surface meteorological conditions than was observed by GRACE. These behaviors can be seen in the central Africa where OL TWS increased more than GRACE TWS during the 2006–2010 wet period and decreased more than GRACE in the following dry period.

Figure 2 shows that GRACE data assimilation was effective in bringing modeled TWS closer to GRACE observations in most regions and under most conditions by the design of data assimilation. In the Amazon

observations for correcting the forcing data. Regardless of the cause for these discrepancies, data assimilation was unable to move modeled TWS toward GRACE TWS in the northern Africa (Figure 2) because very low precipitation causes a small ensemble spread and hence underrepresented model errors.

In contrast, data assimilation was effective in bringing simulated TWS close to GRACE observations in the North China Plain, where pumping for irrigation has caused a significant regional groundwater decline (Feng et al., 2013) and is not simulated by CLSM. GRACE TWS reflects that decline as a persistent decreasing trend from 2004 to 2016, while OL TWS only shows a decreasing trend during the period (2004–2007) when precipitation decreased.

To examine the impact of GRACE data assimilation at the global domain, Figure S2 maps the temporal standard deviation of nonseasonal monthly TWS anomalies, that is, with their seasonal cycle removed, from CLSM OL, GRACE data assimilation, and GRACE, as well as that of monthly ECMWF precipitation anomalies during 2003–2016. The largest standard deviations of precipitation are in the tropics where precipitation variability contributes significantly to the leading mode of variability in global precipitation (Dai & Wigley, 2000). The OL TWS also shows higher standard deviation in those areas (note the different color scales for the top and the lower three panels). In wetter and warmer climates where ET is energy-limited, more precipitation means higher TWS and thus the strong correlation between those two variables. OL TWS also displays large standard deviations across most of the land around 60°N, where seasonal snowpack is a major component of TWS (Xia et al., 2017). In general, the temporal standard deviations of observed TWS are much smaller, due in part to the fact that the effective spatial resolution of GRACE data is coarse (around 150,000 km²). Another part of the explanation is that CLSM-simulated groundwater responds to precipitation variability strongly as discussed earlier. GRACE TWS exhibits its largest temporal standard deviation in the Canadian archipelago due to the persistent melting of glaciers and ice caps associated with global warming. Because CLSM does not simulate permanent snow and ice cover, it did not reproduce these trends. In most of the rest of the world, the temporal standard deviation of DA TWS was smaller than that of OL TWS and larger than that of GRACE TWS while retaining the spatial details of OL TWS.

5.2. Groundwater Storage

By design, data assimilation brings simulated TWS closer to GRACE-observed TWS, but the impact on simulated groundwater storage depends on the ability of the model and the ensemble smoother (the covariance matrix) to separate groundwater from other TWS components. The independent evaluation using in situ groundwater was then necessary to assess the performance of the model parameterization and the DA system. CLSM-simulated nonseasonal groundwater storage anomalies at the grid cell closest to each observation well were extracted for location-specific analyses. Because GRACE data represent large-scale TWS variability, we also averaged groundwater time series from all well locations across each region (as were the in situ observations) to assess the impact of GRACE data assimilation at the regional scale. Spatial averaging, which has been used in previous studies on in situ soil moisture and groundwater (Bhanja, Rodell, et al. 2017; Brookfield et al., 2018; Eltahir & Yeh, 1999; Li et al., 2015), facilitates examination of the impact of climate on GRACE data assimilation. Although the wells are not evenly distributed in each region or basin, we chose not to use area-weighted averaging as used in Rodell et al. (2007) because it can introduce uncertainty when unrepresentative wells are heavily weighted, especially in those regions with few wells.

5.2.1. Evaluation at the Regional Scale

5.2.1.1. The U.S.

Figure 3 shows that regionally averaged, nonseasonal groundwater storage anomalies from OL correlate well with the in situ data in the eight U.S. regions, with correlation coefficients near and above 0.5 in all except Long Island and Red River-Lower Mississippi (Red-LM; Table 1). CLSM was never calibrated using in situ groundwater data; thus, the strong correlations reflect the facts that (1) precipitation and other forcing fields are well constrained in the input forcing data and (2) ET, which, along with precipitation, has the largest impact on groundwater recharge at seasonal to interannual scales (Eltahir & Yeh, 1999; Perez-Valdivia et al., 2012), is reasonably simulated by CLSM. On the other hand, CLSM is not well configured to simulate groundwater recharge where the regional water table is deep (Table S1), such as in the Red-LM basin. In Long Island, where groundwater is the primary source of freshwater (Busciolano, 2002), it is possible that the in situ data were directly affected by groundwater abstraction, despite our efforts to exclude such wells. In addition, the 0.25° resolution forcing data may not have captured the temporal variability of precipitation

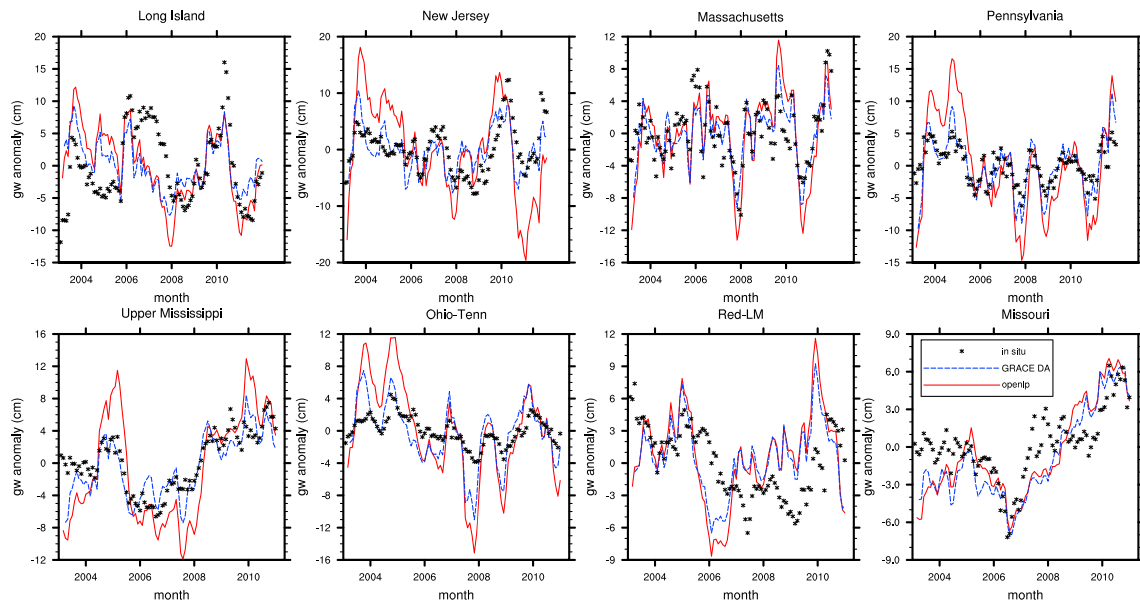


Figure 3. Monthly nonseasonal groundwater storage anomalies from the OL, GRACE DA, and in situ data in the four Mississippi subbasins and four northeast U.S. regions.

Table 1

Root-Mean-Square Errors (RMSE, cm) and Coefficients of Correlation (Cor) Between Region-Averaged (Except for Kin Kin and Maiduguri) CLSM Groundwater Storage Anomalies and In Situ Data

U.S.								
	LI	NJ	MA	PA	Up-Mis	Ohio-Tn	Red-LM	Missouri
RMSE	5.42(5.86)	3.66(7.27)	2.60(3.5)	2.47(5.49)	2.16(4.35)	2.8(4.45)	3.97(4.67)	2.22(2.42)
Cor	0.41(0.47)	0.60(0.49)	0.75(0.73)	0.85(0.81)	0.84(0.81)	0.76(0.88)	0.22(0.21)	0.82(0.77)
Brazil								
	Parana	Sao Francisco	Atlantico Sul		Amazonas	Uruguai	Tocantins	
RMSE	4.95(7.07)	3.98(9.34)	5.21(7.89)		4.22(5.74)	2.81(2.56)	5.83(18.32)	
Cor	0.67(0.46)	0.80(0.74)	0.63(0.30)		0.65(0.55)	0.91(0.93)	0.69(0.47)	
Asia								
	Southern India				North China Plain			
RMSE	3.90 (3.98)				11.32(12.09)			
Cor	0.69 (0.54)				0.83(0.61)			
Australia								
	SW Australia				NE Australia		SE Australia	
RMSE	2.36(2.73)				7.31(7.63)		7.97(9.04)	
Cor	0.29(0.55)				0.65(0.68)		0.72(0.39)	
Europe								
	Rhine				The Netherlands			
RMSE	2.06(2.56)				3.12(4.10)			
Cor	0.50(0.64)				0.40(0.24)			
Africa								
	Uganda		Kin Kin			Maiduguri		
RMSE	5.34(17.20)		6.71(9.93)			11.11(18.71)		
Cor	0.56(-0.05)		−0.05(0.01)			0.63(0.55)		
Average over all								
					wells		regions	
RMSE					7.60(8.40)		4.34(6.74)	
Cor					0.33(0.27)		0.65(0.56)	

Note. Numbers in parentheses are for the open loop simulation. Abbreviations for the U.S. regions are provided in Table S1.

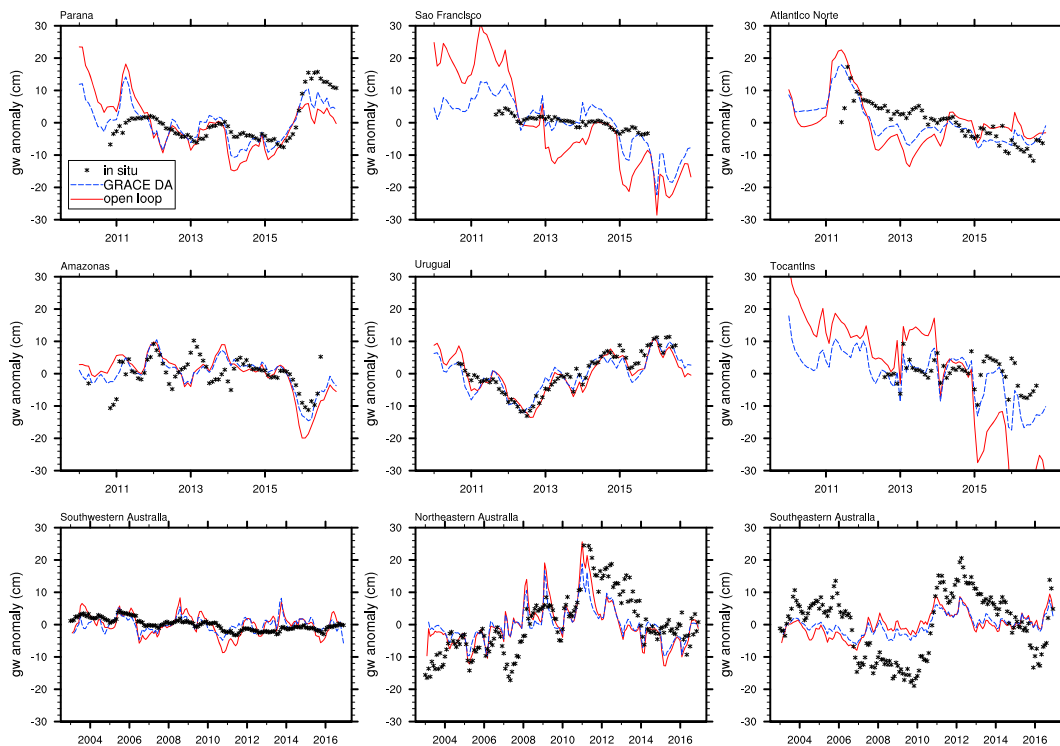


Figure 4. Same as Figure 3 but for the six hydrological basins in Brazil (upper two rows) and the three Australian regions (bottom row).

in Long Island, which has a maximum north-to-south width of only 37 km. Indeed, Li and Rodell (2014) showed that the correlation between CLSM and the in situ groundwater storage anomalies was substantially improved in Long Island when CLSM was forced with a higher-resolution meteorological data set. Table 1 shows that GRACE data assimilation decreased the root-mean-square errors (RMSE) in all eight U.S. regions. In several of those regions (e.g., Pennsylvania; see Figure 3) the improvement partly or largely results from a reduction of the dynamic range of TWS, and hence groundwater, by GRACE data assimilation, making the latter more consistent with the in situ observations. Further, GRACE data assimilation improved the correlation between modeled and in situ groundwater time series in all U.S. regions except Ohio-TN and Long Island. Note that improved correlation is not an implied outcome of a Kalman filter or smoother as the ensemble update aims to minimize estimation errors only.

5.2.1.2. Brazil

GRACE data assimilation also reduced the dynamic range of simulated groundwater storage in Brazil (Figure 4), especially in the Sao Francisco and Tocantins basins where OL groundwater storage declined significantly during 2011–2015. Examining the forcing data and model output reveals that enhanced precipitation intensity led to increased surface runoff and thus reduced groundwater recharge. Whether or not this change in precipitation was real, the result demonstrates the effectiveness of GRACE data assimilation in constraining the interannual variability of simulated groundwater storage and improving the correlation with in situ data (Table 1). Figure 4 shows that in situ groundwater generally exhibits less high-frequency variability than modeled groundwater in Brazil. A possible explanation is that the thick unsaturated zone above the water table (Table S1) may filter out high-frequency meteorological variability.

5.2.1.3. Australia

The OL simulation generally captured the multiyear temporal variability of groundwater as observed in the southwestern and northeastern Australian regions (Figure 4). In southeastern Australia, which was affected by the Millennium Drought from 2001 to 2009 (van Dijk et al., 2013), in situ groundwater was exceptionally low during 2007–2010, while CLSM indicated a minimum in late 2006. Groundwater may have been affected by abstraction for irrigation in the area, especially during the drought (van Dijk et al., 2013), which CLSM would not have captured. Still, considering that the drought continued through 2009, the OL results suggest errors in the forcing data. GRACE TWS was the lowest in 2009–2010 (not shown), and accordingly, GRACE

data assimilation reduced simulated groundwater storage until that time, yet it failed to make 2009–2010 the driest. Overall, data assimilation led to improved correlation and decreased RMSE (Table 1).

Similarly, CLSM failed to simulate the groundwater minimum of northeastern Australia in 2007, likely due to its inability to account for groundwater withdrawals. In southwestern Australia, the response of observed groundwater to changes in precipitation is muted, including during the 2007 and 2011 drought periods. This behavior suggests that the aquifers are semiconfined or the permeability is low, which would reduce groundwater sensitivity to surface meteorological conditions. Indeed, the geological formation of the Southern Perth Basin where these wells are located includes layers of low-permeability sediments such as shales and clays (https://www.water.wa.gov.au/_data/assets/pdf_file/0020/4961/83807.pdf). Further, the specific yield values obtained from the PCR-GLOBWB are 0.05 or less for this region, which may be an indication of semiconfined conditions.

5.2.1.4. Eurasia

In the North China Plain, where groundwater supports 70% of irrigation (Liu et al., 2011), in situ groundwater decreased during 2006–2011 (Figure 5). As expected, the OL simulation does not reflect this long-term depletion because CLSM does not simulate anthropogenic effects. Data assimilation induced a slight decreasing trend in groundwater that is aligned with that of GRACE TWS (Figure 2). Owing in part to this, the DA results are much more strongly correlated with the in situ data (Table 1), despite the RMSE remaining high. Observed groundwater storage increased substantially during 2012–2013, which was associated with increase in heavy precipitation (Figure 2). The upper shallow aquifers of the North China Plain consist of Quaternary sands and gravels, which are conducive to recharge (Liu et al., 2011). These hydrogeological conditions are not represented in CLSM; hence, simulated groundwater does not react strongly enough to precipitation changes. Döll et al. (2014) also attributed overestimation of groundwater depletion in the North China Plain to underestimation of groundwater recharge.

Table 1 shows that GRACE data assimilation decreased RMSE in Rhine, the Netherlands, and Southern India. In Southern India, observed groundwater does not respond strongly to the wet meteorological conditions in 2007, 2008, and 2011 (based on precipitation data, which are not shown). It is possible that the quarterly measurements (see supporting information, S1, and Bhanja, Rodell, et al. 2017) missed the annual maxima, which would be enhanced in a monsoon-dominated climate.

5.2.1.5. Africa

Because there are less than 2 years of in situ data from the wells located in Chad (Kin Kin) and Nigeria (Maiduguri), groundwater storage anomalies are compared and evaluated relative to their temporal mean rather than their monthly mean (Figure 5). Table 1 shows that GRACE data assimilation decreased RMSE at both wells but it did not improve correlation at Kin Kin, where the modeled seasonal cycle was out of phase with the in situ observations. At Maiduguri, the seasonal cycle of groundwater is better simulated and data assimilation was able to improve the correlation even more. Despite the deeper water table depth (Table S1), the seasonal phase of measured groundwater in Maiduguri leads that of Kin Kin. Interaction with surface water may be a factor as Kin Kin is located between the Chari and Logone rivers, which provide 90% of inflow for Lake Chad (Buma et al., 2016). The dynamic range of observed groundwater storage is much smaller than that of CLSM groundwater (note the different y axis scales in the two lower right plots of Figure 5), which may be attributed to the small specific yield, 0.02, prescribed based on Guideal et al. (2011).

In Uganda, where substantial recharge often follows heavy precipitation in the fractured crystalline aquifers (Nanteza et al., 2016), CLSM (OL) correctly produced groundwater increases during 2007–2008 when precipitation intensified (Figure 5). However, the amount of increase was overestimated, which is consistent with that of TWS in the region (see Figure 2, the central Africa panel). GRACE data assimilation reduced the dynamic range of CLSM groundwater and improved the interannual variability, consequently decreasing RMSE and improving correlation considerably (Table 1).

5.2.2. Evaluation at the Grid Scale

To examine the impact of GRACE data assimilation on anomaly time series of groundwater at the scale of the model grid (0.25°), Figure 6 plots the difference between DA and OL RMSE versus the difference in correlation at all well locations. GRACE data assimilation decreased RMSE (negative Diff in RMSE) of CLSM modeled groundwater at most well locations. However, improvements in correlation were less prevalent, especially in India, the U.S., the Rhine, the Netherlands, and Australia. Figure 6 also shows that an increase in correlation generally correlates positively (represented by the red regression line) with a decrease in

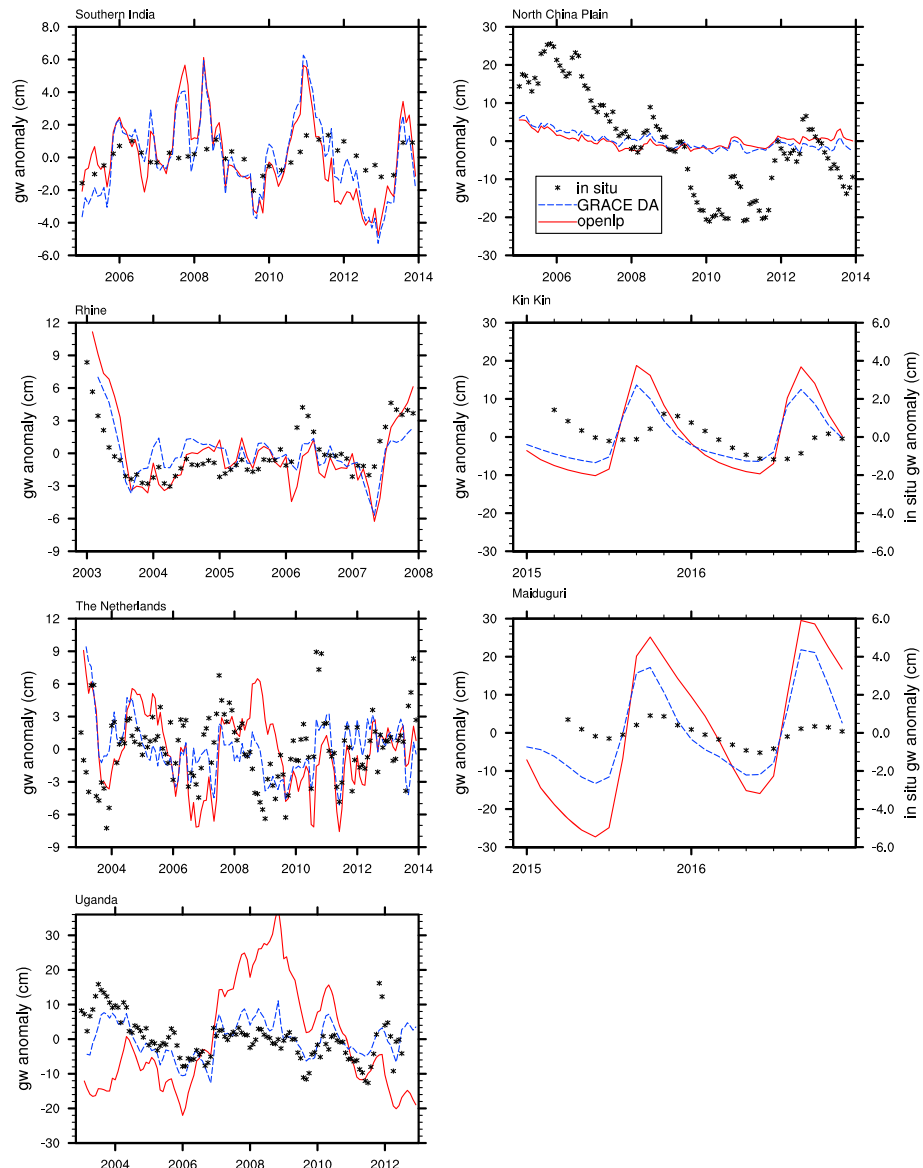


Figure 5. Same as Figure 3 but for Southern India, the North China Plain, the Rhine, the Netherlands, and Uganda, and seasonal groundwater storage anomalies at Kin Kin and Maiduguri. Note that in situ groundwater at Kin Kin and Maiduguri has a different y axis scale than CLSM groundwater.

RMSE. The region dependency of the linear relationship may be affected by the temporal variability of groundwater in each region. For instance, the steep regression line in the North China Plain is due to the fact that correlation is sensitive to the long-term trend, and thus, a small decrease in RMSE may be associated with a large increase in correlation.

Figure 6 also shows that the differences in RMSE and correlation for region-averaged groundwater are within the range of those at the point scale, suggesting that improvements at well locations are closely associated with regional improvements, which makes sense given the coarse resolution of the GRACE data. This is further confirmed in Figure S3, which shows that locations where GRACE data assimilation did not decrease RMSE (represented by blue and black circles) are scattered in each region. On average, GRACE data assimilation reduced RMSE of groundwater storage anomalies by 36% (regional scale) and 10% (point scale) and improved correlation by 16% (regional scale) and 22% (point scale, Table 1). Larger improvement in RMSE at the regional scale is consistent with the coarse resolution of the GRACE data. On average, CLSM OL groundwater time series correlate poorly with the in situ time series at the point scale (Table 1) due to the

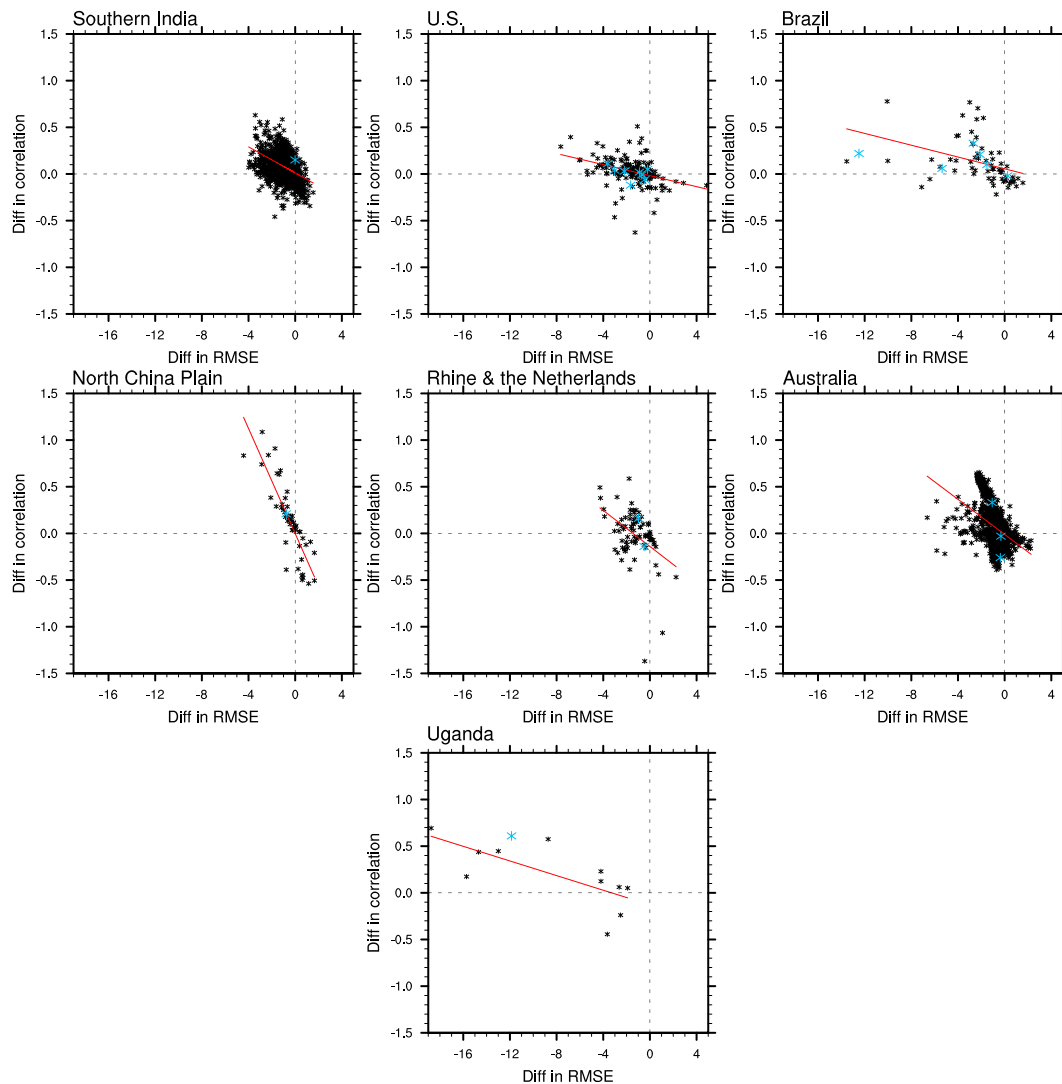


Figure 6. Scatterplots of RMSE differences between GRACE DA and the OL versus correlation differences between DA and OL at the well locations (black asterisks) and at regional scale (blue asterisks). The red lines represent linear regression based on statistics at well locations only.

large-scale nature of the forcing data, which sets a low bar for improvement through data assimilation. Note that uncertainty associated with specific yield does not affect the point-scale correlations but it may impact RMSEs calculated at regional and point scales and the correlations at the regional scale.

5.3. Evaluation Using GRDC Low Flow

Figure 7 shows the correlation between GRDC annual low flow and CLSM OL (x axis) and DA (y axis) annual low groundwater storage (averaged over each basin), both of which were derived based on monthly values. OL low groundwater exhibits weak correlations with low flow in several high-latitude basins (Kolyma, Ob, Slave, Yukon, Makenzie, Thelon, Severnaya, marked in blue) where both low-flow and low groundwater storage exhibit large interannual variability, and thus, the correlation may be more sensitive to the small number of annual lows (≤ 15). OL annual low groundwater also exhibits weak correlation with low flow in the Ubangi river basin (marked in red) where the peneplain terrain lengthens groundwater travel time to the gauge location (Aich et al., 2014) and thus, the low correlation may be affected by the short evaluation period.

GRACE data assimilation, on average, improved the correlation between CLSM low groundwater storage and GRDC low flow. This is because groundwater base flow is a major component of low flow, especially in large river basins (Orlova & Branfireun, 2014), and GRACE captured changes in annual minimum TWS.

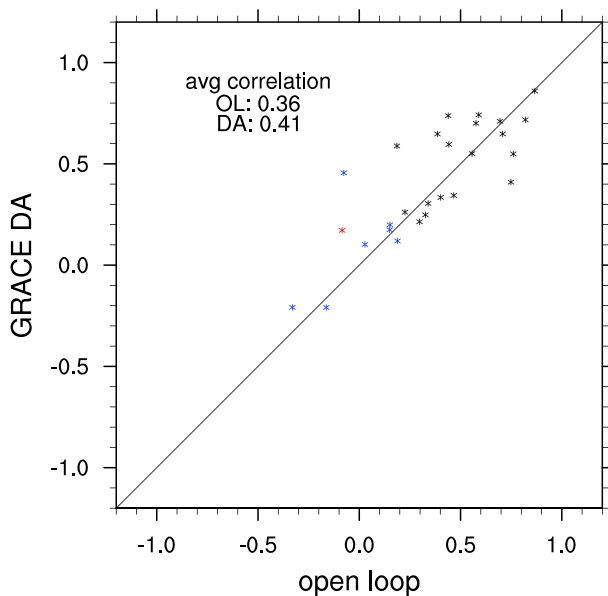


Figure 7. Correlation between GRDC low-flow and basin-averaged CLSM OL low groundwater (x axis), DA low groundwater (y axis). The red mark represents the Ubangi basin, and blue marks represent the Kolyma, Ob, Slave, Yukon, Makenzie, Thelon, and Severnaya river basins.

Thawing of permafrost in northern high-latitude regions is not simulated by CLSM, but its effects, such as increase in runoff and groundwater recharge, are detectable by GRACE (Muskett & Romanovsky, 2009; Velicogna et al., 2012) and thus may be reflected in DA groundwater. In addition, changes in precipitation and loading and unloading of seasonal snow mass, which are reflected in the forcing data or simulated by CLSM, also affect what GRACE observes (Muskett & Romanovsky, 2009; Velicogna et al., 2012). Due to the shortness of the GRACE period, these statistics based on annual low values are subject to change and should be reexamined after several years of GRACE Follow On data become available for data assimilation.

5.4. Evaluation Across Hydrogeological Settings

Figures 8(a) and (b) show the differences in RMSE and correlation between DA and OL at well locations (also shown in Figure 6) as a function of log-permeability (negative values are due to the log-transformation) from Gleeson et al. (2014). Most in situ wells are located in regions with medium permeability (Figure S1). When averaged over each permeability category, only the mean differences in correlation show a weak negative relationship (the significance level, α , is provided in the figure) with permeability (Figures 8c and d), indicating that GRACE data assimilation improved the correlation more in lower permeability zones.

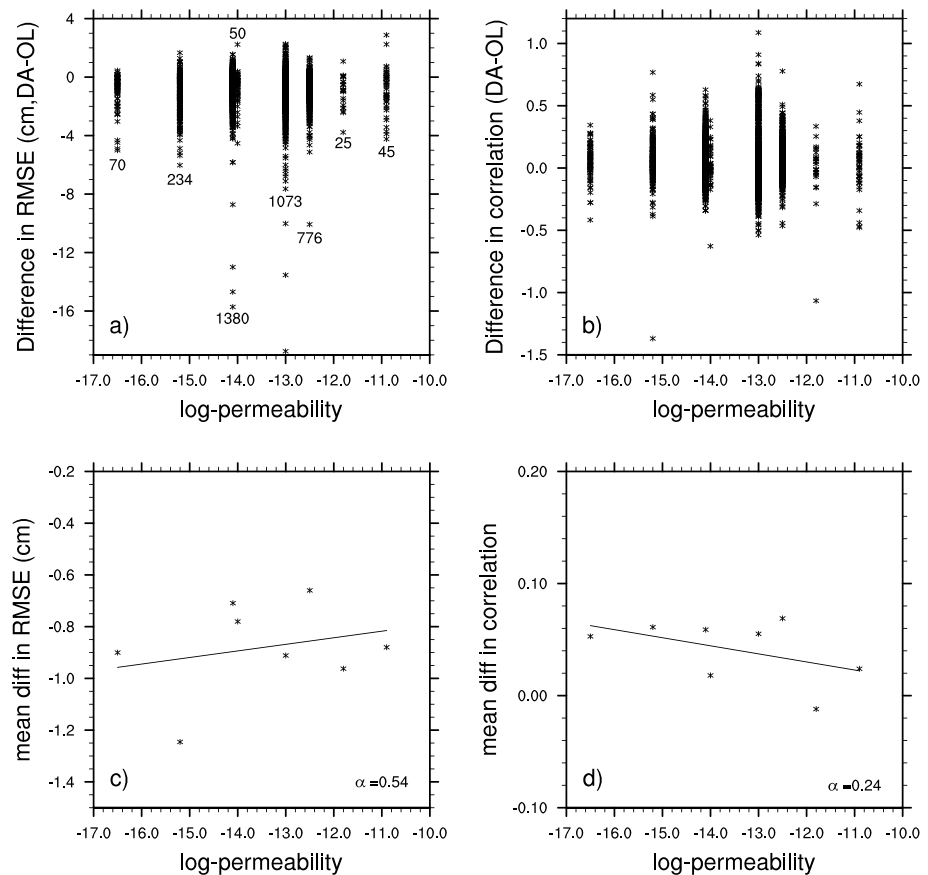


Figure 8. Differences in RMSE and correlation (DA-OL) at well locations (a and b) and averaged differences in RMSE and correlation over each permeability category (c and d) as a function of Gleeson permeability. α represents the significance level of regression lines. The numbers in (a) represent the number of wells in each permeability category.

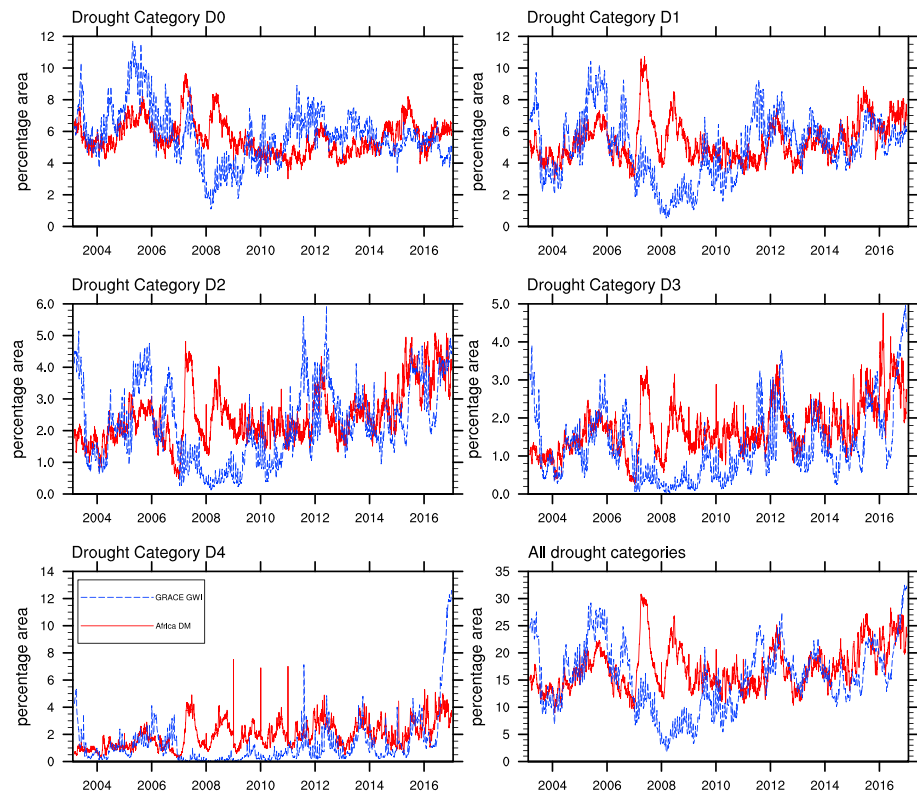


Figure 9. Percentages of drought areas estimated by GWI and African FDM for the five drought categories, D4 (exceptional drought), D3 (extreme drought), D2 (severe drought), D1 (moderate drought), D0 (abnormally dry), and the sum of the five categories.

Similar analysis did not find that RMSE and correlation of OL groundwater are related to the permeability (not shown).

Since CLSM does not use a permeability parameter, this apparent linear relationship suggests a link between the permeability data set and CLSM bedrock depth, which has the largest impact on the temporal variability of simulated groundwater storage among all CLSM parameters. Indeed, CLSM bedrock depths averaged over each Gleeson permeability category exhibit a negative correlation with permeability (Figure S4), indicating that deeper bedrock depths correspond to lower permeability. This relationship is logical given that the spatial pattern of CLSM bedrock depths is loosely based on geology, climate, and topography (Koster et al., 2000).

Note that CLSM uses a saturated hydraulic conductivity parameter only for calculating base flow (Koster et al., 2000) and its impact on the temporal variability of groundwater is much smaller than that of bedrock depth. Figure S1 shows that the CLSM hydraulic conductivity data set (converted to log-permeability for comparison), derived based on soil texture and pedotransfer functions (Koster et al., 2000), is not correlated with the Gleeson permeability.

5.5. Evaluation of Drought Indices

To evaluate the ability of the GRACE-based GWI to properly detect droughts under different climate conditions, we compare the GWI with other regional drought indicators. Considering that most regional indicators emphasize agricultural drought (section 3.6), the comparison also demonstrates the value of the GWI for identifying hydrological and groundwater drought. Figure 9 shows that the average drought areas in each of the five categories estimated by the GWI and the African FDM are similar, close to the prescribed probabilities stated in section 3.6, but the categorical drought areas identified by the two indicators do not agree consistently over time. In particular, the African FDM reported elevated drought conditions during 2007–2008, while GWI indicated much less drought. Heavy rains (Figure 2) in central Africa during that period

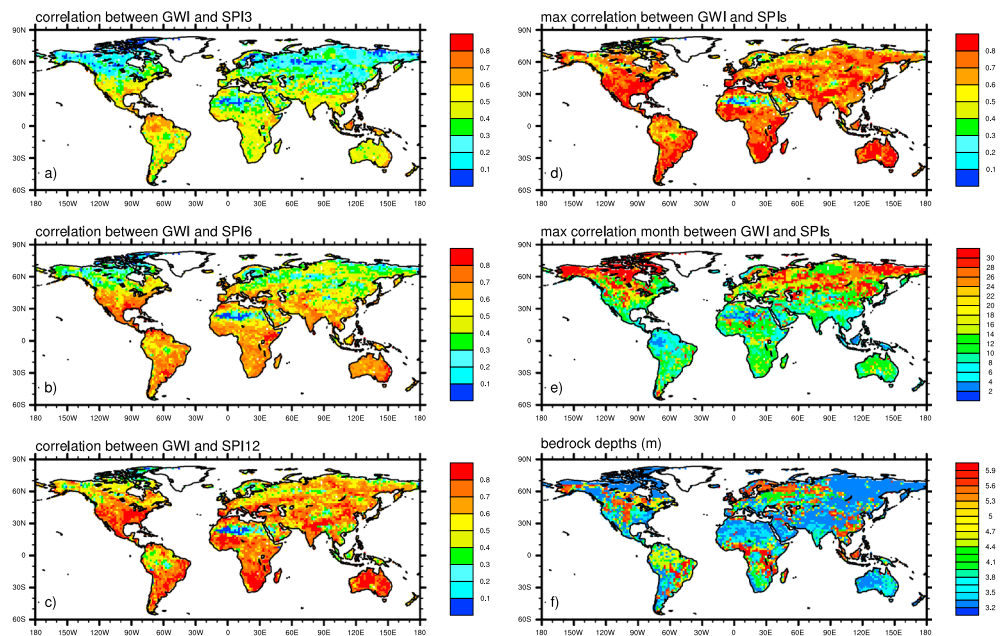


Figure 10. Correlation between monthly GWI and SPI3, SPI6 and SPI12 (left column), and maximum correlation between GWI and the SPIs, month of maximum correlation, and CLSM bedrock depths (right column).

led to increased groundwater storage. The 1-m root zone soil moisture, which is the basis of the African FDM, has a shorter *memory* than groundwater and thus decreased more quickly during that period.

On the other hand, USDM regularly estimated a higher percentage drought area than the GRACE GWI in all but the D4 category (Figure S5). USDM depends in part on subjective consideration of data from multiple sources, and thus, it is not constrained by the target probabilities for each category. Overall, USDM indicated drought about 40% of the time averaged over the entire domain, well above the 30% threshold for drought (section 3.6). Nevertheless, drought areas identified by the USDM and GWI behaved similarly in the D1 to D3 categories including the increases in 2006–2008 and 2012–2016. The temporal variations of their D0 drought areas differed significantly, especially in 2008 and 2014–2016 when USDM indicated increasing drought areas but GWI suggested otherwise. The latter can be attributed to the lagged response of groundwater to surface meteorological conditions. GWI predicted more exceptional drought (D4) than USDM after 2013, which was due to the historically low GRACE TWS values (not shown) in the western U.S.

Similar to USDM, the Canadian DM is less constrained by the prescribed drought probabilities and reported no D4 (exceptional) drought (Figure S6) over the study period but more abnormally dry conditions (D0). Overall, the two indicators display similar temporal variability. The temporal (in)consistency between groundwater drought and other types of drought may also be affected by climate and hydrogeological conditions, and spatial variability thereof.

5.6. Temporal Variability of Groundwater

Evolution of groundwater drought is affected by surface meteorological conditions, soils and vegetation, water table depth, and subsurface hydrogeological properties. To quantify the temporal variability of CLSM simulated groundwater storage, we calculated the correlation between GWI (derived from the Princeton-forced climatology run) and the SPI (derived from Princeton precipitation), which represents meteorological drought. The use of the longer Princeton-forced simulation (as opposed to the GRACE data assimilation run) provides more robust statistics and more insight into the relationship between groundwater drought and large-scale climate variability.

Figure 10 shows that CLSM-derived GWI exhibits a strong correlation with the 3-month SPI (SPI3) in a few tropical and subtropical regions including northern South America, east central Africa, Indonesia, and southeastern Australia, where the El-Niño Southern Oscillation is known to have the largest impact on precipitation (Dai & Wigley, 2000). GWI was weakly correlated with SPI3 in high-latitude regions where

groundwater recharge is mainly driven by spring snowmelt (Perez-Valdivia et al., 2012) and where ET is minimal, leading to less seasonal variability in groundwater storage. As the SPI averaging period is increased from 3 months to 12 months, the correlation between SPI and GWI increases in most regions where the influence of the El-Niño Southern Oscillation is not dominant, reflecting the lagged response of groundwater to atmospheric forcing. In the Sahara Desert, where groundwater recharge is nearly zero, a low correlation is observed at all timescales. In general, GWI is best correlated with a roughly 12-month SPI for most global land areas (Figures 10d and 10e), with much longer SPI integration periods in the cold high-latitude regions and shorter integration periods in the tropics. These results are consistent with those based on in situ groundwater data in the U.S. (Russo & Lall, 2017) and India (Asoka et al., 2017).

As indicated earlier, temporal variability of groundwater may also be influenced by hydrogeological conditions such as hydraulic conductivity and the depth to the water table. CLSM does not represent complex hydrogeological processes, but it does include a spatially varying *bedrock depth* parameter, which exerts strong control on the timescales of simulated groundwater. In general, deeper bedrock leads to a deeper water table and thus more low-frequency variability in groundwater. For example, Figure 10e shows that GWI in the U.S. Great Plains and northwestern Europe, where CLSM bedrock is particularly deep, has longer maximum SPI correlation times. However, the effect of bedrock depth on groundwater temporal variability may be superseded by that of precipitation and ET. For instance, despite deep bedrock in central Africa, southeast China, and Indonesia, GWI correlates strongly with short-scale SPIs because heavy precipitation in these regions is associated with enhanced infiltration and recharge. In these regions, increased groundwater storage delays the onset of groundwater drought, which is why GWI indicated substantially less drought area than the African FDM during 2007–2008 (Figure 9). In Canada, where the bedrock depth is relatively uniform, the spatial extent of groundwater drought is mainly determined by surface meteorological conditions, and thus, in a given area, the temporal variability of groundwater drought is similar to that of agricultural drought (Figure S6).

Note that our GRACE-based GWI differs fundamentally and exhibits different characteristics from indicators based on GRACE TWS alone (e.g., Thomas et al., 2014; Zhao et al., 2017), which represent drought conditions in the entire surface-soil-aquifer profile, including snow. For instance, the GRACE TWS-based indicator of Zhao et al. (2017) exhibited the strongest correlation with the Standard Precipitation Evapotranspiration Index at 12-month or shorter timescales in northern Eurasia, northeastern China, and the Himalayas where snow hydrology dominates temporal variability of TWS. GWI shows the strongest correlation with SPIs at the 26-month or longer timescales in those areas (Figure 10). In addition, these TWS-based indicators, along with those derived by estimating groundwater time series from GRACE TWS using auxiliary data (e.g., Thomas et al., 2017), are limited to coarser spatial and temporal (monthly) scales due to lack of downscaling. Just as importantly, while a data assimilating model enables continued estimation of groundwater variations across satellite gravimetry data gaps and up to near real time by making use of meteorological forcing data, indicators derived from GRACE data without data assimilation cannot overcome data gaps or latency, and hence are poorly suited for operational applications that require timely information.

6. Discussions and Conclusions

Data assimilation through the ensemble Kalman smoother enables vertical disaggregation and spatial and temporal downscaling (to 0.25° resolution and daily intervals in this study) of GRACE TWS data. For the purpose of drought monitoring, it has the added benefit of bridging temporal gaps in the GRACE (and GRACE Follow On) data set and extending the results to near real time.

GRACE data assimilation has a large impact on the interannual variability of modeled TWS in the tropics, subtropics, and northern Eurasia. CLSM-simulated (open loop) TWS differs considerably from GRACE TWS in these regions due to differences between the modeled and real-world responses to strong interannual variability of precipitation, including the partitioning between ET, surface runoff, and recharge. The discrepancies may also be caused by errors in the reanalysis-based meteorological data used to force the model. Given that groundwater storage changes influence the rate of base flow, GRACE data assimilation may be beneficial when using LSM output for short-term to seasonal streamflow forecasting, especially considering that it increased the correlation between annual low flow and CLSM low groundwater at many GRDC

stations. On the other hand, as shown in Li et al. (2012), large increments (TWS updates) often lead to imbalances in the simulated water budget (simulated TWS changes equaling the net of precipitation, ET, and runoff). For instance, in central Africa (Figure 2), GRACE data assimilation reduced simulated TWS during 2006–2010, which in turn decreased ET and runoff, hence an imbalance in the water budget that did not exist in the open loop. Changing that outcome would require constraining the fluxes (such as through flux data assimilation).

Evaluation using in situ groundwater showed that GRACE data assimilation had strong positive impacts on simulated groundwater storage time series in several regions and climates around the world, with average RMSE reduced from 8.4 to 7.6 cm (point scale) and from 6.7 to 4.3 cm (regional scale), and correlation improved from 0.27 to 0.33 (point scale) and from 0.56 to 0.65 (regional scale; Table 1). Consistent with its impact on TWS, GRACE data assimilation led to larger improvements in simulated groundwater in regions with large interannual variability, such as Brazil, the Netherlands, and Uganda. These improvements, based on a much larger number of in situ wells covering more continents than those used in previous studies, are strong indications that GRACE captured the interannual variability of groundwater storage changes, confirming its value in helping to overcome the scarcity of in situ groundwater observations. These positive impacts were further demonstrated by the improved correlation, averaged over 27 stations, between simulated annual low groundwater storage and GRDC low flow. Compared to model calibration using GRACE data that require auxiliary information to isolate groundwater (Lo et al., 2010; Sun et al., 2012), GRACE data assimilation has the advantage of constantly adjusting the simulated TWS (and its components) to be consistent with GRACE observations, while GRACE-based calibration may only constrain the dynamic range of simulated TWS with little impacts on its interannual variability.

In this study GRACE data assimilation generally increased the correlation between modeled and in situ groundwater, but not as consistently as it decreased RMSE. In the case of Kin Kin, where the simulated seasonal cycle of groundwater storage was out of phase with that of the in situ data, GRACE data assimilation decreased RMSE without improving correlation at all. These results reflect the nature of Kalman filters, which are designed to minimize estimation errors at the time of update, without consideration for the temporal variability of the simulated variables. Correlation may also be strongly influenced by long-scale variability in the data such as a secular trend, as seen in the North China Plain. Note that we did not test the significance of the improvements in correlation because groundwater anomalies exhibit strong autocorrelation, while the commonly used statistical methods such as the Student's *t* test assume sample independence. Approaches for estimating an effective sample size often yield inconsistent results (Trenberth, 1984), and more importantly, the effective sample size cannot be substituted for the degree of freedom used in the Student's *t* test (Thiébaux & Zwiers, 1984). DA and OL groundwater time series are also strongly cross correlated through the update process, equation (1).

The large number of multiyear water level measurement records also enabled a more complete assessment of uncertainties in modeled groundwater and their relationship with climate. The larger-than-observed interannual variabilities seen in CLSM-simulated groundwater storage time series generally occurred in regions with large interannual variability in precipitation and may be caused by errors in the ECMWF precipitation data and deficiencies in model physics. For instance, in cases where the 1-m root zone prescribed in the model is unrealistically thin, it will not filter out high-frequency meteorological variability as much as a thicker root zone would. Xia et al. (2017) found that CLSM-simulated groundwater storage in the U.S. exhibited larger dynamic ranges (when seasonality is included) than two other LSMs whose root zones were at least 2 m deep.

On the other hand, evaluation across hydrogeological settings did not yield strong evidence that the performance of CLSM and GRACE data assimilation is correlated with the permeability by Gleeson et al. (2014). This result may be called into question by the limited number of permeability categories (eight). In addition, the statistics, which were calculated based on nonseasonal groundwater storage anomalies, may mainly reflect long-term groundwater variability while hydrogeological properties such as permeability may have a stronger impact on short-term (hourly to daily) groundwater variability. This issue should be reexamined in future studies when in situ groundwater data at higher temporal intervals are available.

CLSM-simulated groundwater storage is bounded by the soil profile water storage capacity, which is the product of prescribed bedrock depth and porosity. As a result, CLSM cannot replicate long-term, intense

groundwater abstraction. For instance, based on estimated depletion rates (Döll et al., 2014), simulating groundwater withdrawals with the current parameterization would leave the soil profiles empty after about 10 years of simulation in heavily irrigated areas like the Central Valley of California, northern India, and the North China Plain. Prescribing substantially deeper bedrock to accommodate rapid groundwater depletion can have unintended consequences on simulated base flow and other fluxes (not shown). This is less of an issue in models such as WaterGAP (Döll et al., 2014) and PCR_GLOBWB (Sutanudjaja et al., 2018) in which groundwater storage changes are computed without the soil profile capacity constraint. Compared to WaterGAP, PCR_GLOBWB, and the dynamic flow model, ParFLOW (Kollet & Maxwell, 2008), CLSM also lacks explicit schemes for calculating moisture fluxes between different water stores such as groundwater recharge, which is needed for coupling with a dynamic model to simulate lateral groundwater flow (de Graaf et al., 2017; Reinecke et al., 2018). Overcoming these limitations would require substantial changes to the model structure and physics.

In addition, like many other LSMs, CLSM lacks a module for simulating surface water (rivers and streams) dynamics (Xia et al., 2017). Consequently, the contribution of surface water to TWS is assumed to be either insignificant or encompassed by the groundwater storage changes. These assumptions may be problematic in areas with large and dynamic surface water storage such as the Amazon (Getirana et al., 2017). In such regions, an alternative, when optimal simulation of groundwater storage changes is the primary goal, would be to set a larger observation error to decrease the impact of GRACE data assimilation on modeled groundwater.

We conclude that in general and across the world, GRACE data assimilation improves the simulation of groundwater storage variations in comparison with in situ measurements, which lends confidence in applying the results for groundwater drought monitoring. Our analysis showed that CLSM simulated groundwater drought generally lags meteorological drought (represented by SPI) by 12 months, with quicker responses in the tropics and more delayed responses in high-latitude regions, reflecting the impact of climate conditions and hydrogeologic properties on drought propagation to groundwater. Hence, groundwater may not be a good indicator of the onset of drought associated with short-term precipitation deficits and high temperatures (i.e., flash drought). On the other hand, groundwater (and TWS) variations integrate medium-to-long-term meteorological conditions and thus provide a useful indication of the depth and duration of droughts that is more physical than a precipitation index, for example. Further, in a region where the shallow aquifer is in communication with plant roots, streams, and surface waters, a depressed water table likely makes the area more vulnerable to the onset of agricultural and hydrological drought, while an elevated water table provides some resiliency. The current inability of CLSM to simulate groundwater abstraction is less relevant in the context of drought monitoring if abstraction-induced groundwater depletion is considered separately.

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