

# The Application of Multi-mission Satellite Data Assimilation for Studying Water Storage Changes over South America

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## Abstract

1 Constant monitoring of total water storage (TWS; surface, groundwater, and soil moisture) is  
2 essential for water management and policy decisions, especially due to the impacts of climate  
3 change and anthropogenic factors. Moreover, for most countries in Africa, Asia, and South  
4 America that depend on soil moisture and groundwater for agricultural productivity, moni-  
5 toring of climate change and anthropogenic impacts on TWS becomes crucial. Hydrological  
6 models are widely being used to monitor water storage changes in various regions around the  
7 world. Such models, however, comes with uncertainties mainly due to data limitations that war-  
8 rant enhancement from remotely sensed satellite products. In this study over South America,  
9 remotely sensed TWS from the Gravity Recovery And Climate Experiment (GRACE) satel-  
10 lite mission is used to constrain the World-Wide Water Resources Assessment (W3RA) model  
11 estimates in order to improve their reliabilities. To this end, GRACE-derived TWS and soil  
12 moisture observations from the Advanced Microwave Scanning Radiometer - Earth Observing  
13 System (AMSR-E) and Soil Moisture and Ocean Salinity (SMOS) are assimilated into W3RA  
14 using the Ensemble Square-Root Filter (EnSRF) in order to separately analyze groundwater  
15 and soil moisture changes for the period 2002–2013. Following the assimilation analysis, Tropi-  
16 cal Rainfall Measuring Mission (TRMM)’s rainfall data over 15 major basins of South America  
17 and El Niño/Southern Oscillation (ENSO) data are employed to demonstrate the advantages  
18 gained by the model from the assimilation of GRACE TWS and satellite soil moisture products  
19 in studying climatically induced TWS changes. From the results, it can be seen that assimi-  
20 lating these observations improves the performance of W3RA hydrological model. Significant  
21 improvements are also achieved as seen from increased correlations between TWS products and  
22 both precipitation and ENSO over a majority of basins. The improved knowledge of sub-surface  
23 water storages, especially groundwater and soil moisture variations, can be largely helpful for  
24 agricultural productivity over South America.

*Keywords:* South America, Satellite remote sensing, Data assimilation, Hydrological modelling, GRACE, Satellite soil moisture

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## 25 **1. Introduction**

26 South America, with unique ecosystems and a high biodiversity, has extreme geographic  
27 variations and diverse patterns of weather and climate that include tropical, subtropical and  
28 extratropical features (Garreaud et al., 2008). The region is largely under the influence of large-  
29 scale ocean-atmosphere phenomena including mainly El Niño Southern Oscillation (ENSO) and  
30 the North Atlantic Oscillation (NAO), which affects climate and its phases associated with  
31 droughts, floods, and extreme weather events within different parts of the continent (Magrin  
32 et al., 2007; Tedeschi and Collins, 2016). Climate variability throughout South America can  
33 be categorized based on the distance from the equator and the altitude of the area. The  
34 Andes mountain ranges, running along South America’s western side, plays an important role  
35 in tropical as well as subtropical latitudes by keeping dry conditions on the west and moist  
36 conditions on the east (Garreaud et al., 2008). These climate variabilities, e.g., due to the  
37 different climatic zones across the continent and/or large-scale ocean-atmosphere phenomena,  
38 have significant impacts on the continent’s water storages (surface water, groundwater, soil  
39 moisture, and vegetation water). There are other important factors that largely threaten water  
40 resources such as excessive water use, especially for agricultural purposes (Grau and Aide, 2008;  
41 Magrin et al., 2014). Therefore, the study of South America’s water storage changes in light of  
42 the climate change and anthropogenic impacts is necessary for any future water use planning.

43 To study South America’s water storage changes at high spatio-temporal resolutions, hydro-  
44 logical models have come in handy (e.g., Betts et al., 1996; Koster et al., 1999; Döll et al., 2003;  
45 van Dijk, 2010; De Paiva et al., 2013; Getirana et al., 2014), particularly over the regions with a  
46 few ground-based observations such as Venezuela, Ecuador, Chile, and Peru. The applications  
47 of these models are especially important for agriculture and sustainable water managements  
48 (e.g., Bharati et al., 2008; Yu et al., 2015; Kourgialas and Karatzas, 2015). However, in general,  
49 data limitations and other factors, e.g., imperfect modeling and uncertainties of model param-  
50 eters can weaken performances of the models for simulation of hydrological processes (van Dijk  
51 et al., 2011; Vrugt et al., 2013). In this regards, data assimilation provides a unique opportu-  
52 nity to improve model reliabilities (Bertino et al., 2003). This approach integrates additional  
53 observations that have not been considered in those models into their dynamics to constrain its

54 state estimates (Bertino et al., 2003; Hoteit et al., 2012).

55 Data assimilation has been used in different applications, e.g., atmospheric fields (Elbern and  
56 Schmidt, 2001; Schunk et al., 2004; Altaf et al., 2014), oceanic (Bennett, 2002; Lahoz, 2007) and  
57 magnetospheric (Garner et al., 1999) studies. The method has also been applied in hydrological  
58 contexts to increase models' performances for estimating various water compartments (e.g.,  
59 Reichle et al., 2002; Alsdorf et al., 2007; Goncalves et al., 2009; Renzullo et al., 2014; Dillon et  
60 al., 2016; Khaki et al., 2018a,b). The use of models to study hydrological variables over South  
61 America are reported, e.g., in the works of Yates et al. (1997), Chou et al. (2002), Grimson  
62 et al. (2013), and Erfanian et al. (2017), who investigate the application of the models on  
63 hydrological resources, droughts, and water storage changes. In the works above, the limitations  
64 have been that the models have not incorporated remotely sensed hydrological products such as  
65 the Gravity Recovery And Climate Experiment (GRACE) with a large capability of estimating  
66 terrestrial water storage (TWS) changes.

67 The main objective of the present study is, therefore, to use multimission satellite data  
68 products to improve hydrological model estimates of sub-surface water storages over South  
69 America. For this purpose, GRACE-derived TWS and soil moisture observations from the  
70 Advanced Microwave Scanning Radiometer - Earth Observing System (AMSR-E) and Soil  
71 Moisture and Ocean Salinity (SMOS) are assimilated into the World-Wide Water Resources  
72 Assessment (W3RA) hydrological model (van Dijk, 2010). The model has been applied at  
73 different continental and global studies including South America (e.g., van Dijk et al., 2013,  
74 2014; Beck et al., 2016; Schellekens et al., 2017). In terms of observations, several studies  
75 indicate that using GRACE TWS (e.g., Zaitchik et al., 2008; Houborg et al., 2012; Li et al.,  
76 2012; Eicker et al., 2014; Li et al., 2015; Reager et al., 2015; Li and Rodell, 2015; Kumar et  
77 al., 2016; Giroto et al., 2016; Khaki et al., 2017a,b; Giroto et al., 2017; Khaki et al., 2018c)  
78 and satellite soil moisture (e.g., Tian et al., 2008; Renzullo et al., 2014; Dumedah et al., 2015;  
79 Tian et al., 2017; Kolassa et al., 2017) for data assimilation can successfully constrain the  
80 hydrological models simulations. The present study aims at investigating the effectiveness of  
81 multi-satellite data assimilation for studying sub-surface water storage changes using a non-  
82 regional hydrological model. It should be pointed out that although similar studies by the  
83 authors have been undertaken for other regions and using different products (e.g., Khaki et al.,  
84 2017c, 2018d), the main distinction and innovativeness between the current work over South  
85 America and those undertaken by the authors above, is that for the first time, both GRACE

86 TWS and soil moisture products are employed in assimilation over the area. Furthermore, the  
87 contribution of climate variability on South America’s water storage derived from assimilation  
88 using satellite precipitation products is also investigated.

89 Assimilation of GRACE TWS data allows users to consistently separate TWS (since both  
90 model and observation errors are considered) into different water compartments that include  
91 groundwater and soil moisture. This is due to the fact that the W3RA model relies on the  
92 physical processes implemented in the model equations. Besides, GRACE-derived TWS obser-  
93 vations are spatially downscaled using this approach, and therefore, higher spatial resolution  
94 estimations of water storages will be available within the study region (see, e.g., [Schumacher  
95 et al., 2016](#)). Moreover, the application of soil moisture observations in the assimilation can  
96 improve the performance of the process by separately updating model soil moisture estimates  
97 (e.g., [Tian et al., 2017](#)). For the purpose of data assimilation, here, we use the ensemble-based  
98 sequential technique of the Ensemble Square-Root Filter (EnSRF) filtering scheme ([Whitaker  
99 and Hamill, 2002](#)) to integrate GRACE TWS into W3RA. EnSRF, as shown in [Khaki et al.  
100 \(2017a\)](#), is preferred over the traditional ensemble Kalman filter (e.g., [Evensen, 2003, 2007](#);  
101 [Eicker et al., 2014](#)) due to its higher computational speed, simplicity, and independence of  
102 perturbed observations.

103 Following the assimilation step, in-situ measurements are used to assess the performance of  
104 the approach. Furthermore, the study investigates the use of the model to study climate induced  
105 water storage changes by comparing correlations between assimilated and non-assimilated re-  
106 sults with climate variability indicators of the Tropical Rainfall Measuring Mission (TRMM)  
107 rainfall and ENSO ocean-atmospheric couple indicator. For a better discussion, the study  
108 area is divided into 15 major basins selected (Figure 1) based on their importance and large  
109 hydro-climatic effects, which also allow us to spatially have a better analysis. We also apply  
110 principal component analysis (PCA, [Lorenz, 1956](#)) on the TRMM rainfall data, groundwater,  
111 soil moisture results from model over each basin to better understand the spatial and temporal  
112 variations of water storages and their interactions with precipitation. [Frappart et al. \(2013\)](#)  
113 found that PCA modes can better represent spatiotemporal variations in time series compared  
114 to the full signals by separating dominant water mass change signals, especially over South  
115 America (see also [Abelen et al., 2015](#)).

116 In the remainder of this study, first, datasets and method are presented in Section 2. We  
117 then discuss the data assimilation filtering scheme in Subsection 2.5 and provide a detailed

118 explanation of the experimental setup in Subsection 2.6. Results and discussions are provided  
 119 in Section 3, and the study concluded in Section 4.

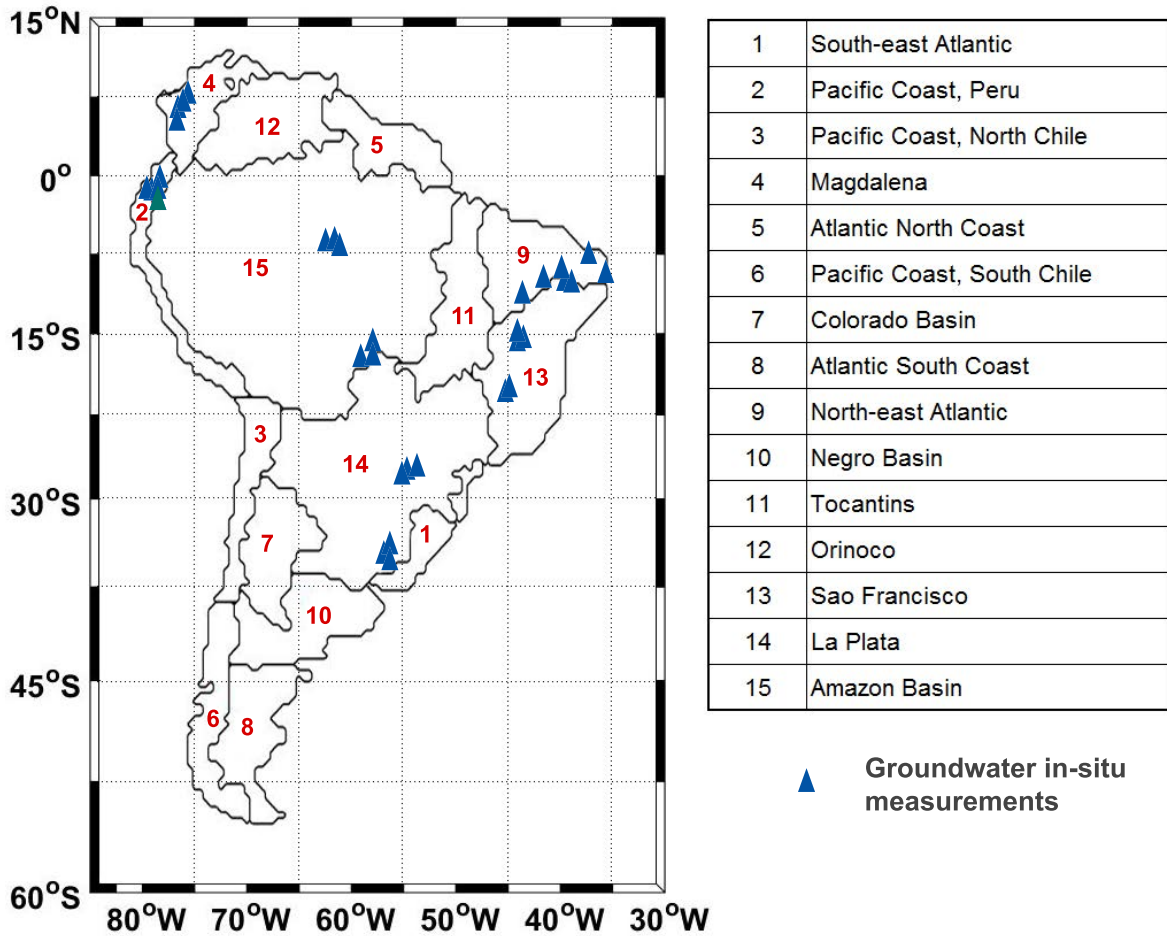


Figure 1: Overview of the study area. The black polygons indicate the 15 river basins considered. These basins are selected according to HydroSHEDS (<http://www.hydrosheds.org/>) classification with small modifications to combine smaller basins and also for a better representation. The basins are sorted according to their areas. Data from in-situ groundwater stations (blue triangles) are used to provide independent validation of the assimilation results.

## 120 2. Materials and methods

### 121 2.1. W3RA hydrological model

122 Vertical water compartments (e.g., soil moisture, groundwater, and surface water)  
 123 of the globally distributed 1°×1° World-Wide Water Resources Assessment system (W3RA;  
 124 <http://www.wenfo.org/wald/data-software/>) model are used to simulate water storage over

125 South America. The model was developed in 2008 by the Commonwealth Scientific and Indus-  
126 trial Research Organisation (CSIRO; Australia) to simulate water storages (van Dijk, 2010). In  
127 terms of forcing data, minimum and maximum temperature, downwelling short-wave radiation,  
128 and precipitation products provided by Princeton University (<http://hydrology.princeton.edu>)  
129 are used. Daily W3RA estimates of top, shallow, and deep root soil layers, groundwater storage,  
130 and surface water storage in a one-dimensional system (vertical variability) are used for data  
131 assimilation (see details in Subsection 2.6).

## 132 2.2. Remotely sensed observations (GRACE, soil moisture and TRMM products)

### 133 2.2.1. GRACE TWS

134 Monthly TWS observations at a  $3^\circ \times 3^\circ$  spatial resolution (suggested by Khaki et al.,  
135 2017b, for data assimilation objectives) derived from the GRACE level 2 (L2) monthly Stokes's  
136 coefficients (following Wahr et al., 1998) up to degree and order 90 are used for the assimilation.  
137 L2 products along with their full error information are obtained from the ITSG-Grace2014  
138 gravity field model (Mayer-Gürr et al., 2014) for the period between 2002 and 2013. Before  
139 converting L2 data into TWS, low degree coefficients of 1 and 2 (C20) are respectively replaced  
140 by those estimated by Swenson et al. (2008) and Satellite Laser Ranging solutions, respectively,  
141 to account for the change in the Earth's center of mass and large uncertainties (e.g., Cheng and  
142 Tapley, 2004; Chen et al., 2007). The DDK2 smoothing filter by Kusche et al. (2009) is applied  
143 to tackle colored/correlated noises in spherical harmonics. In order to reduce leakage effects,  
144 for every one of the 15 basins considered, an isotropic kernel using a Lagrange multiplier filter  
145 proposed by Swenson and Wahr (2002) is applied. This approach reduces short wavelength  
146 effects using Lagrange multiplier to minimize the leakage for a given value of satellite error.  
147 Here, the satellite error is selected based on the acquired GRACE full error covariance matrix.  
148 Khaki et al. (2018e) showed that this filtering technique can effectively reduce leakage errors,  
149 e.g., over Amazon basin. Finally, the mean TWS for the study period is taken from W3RA  
150 and added to the GRACE TWS change time series to obtain absolute values and make them  
151 comparable with model outputs (Zaitchik et al., 2008).

### 152 2.2.2. Satellite soil moisture

153 In addition, soil moisture observations from the Advanced Microwave Scanning Ra-  
154 diometer for EOS (AMSR-E), between 2002 and 2011, and ESA's Soil Moisture Ocean Salinity  
155 (SMOS) Earth Explorer mission, between 2011 and 2013, are used in the data assimilation to

156 update model soil moisture variabilities. The AMSR-E measurements are correlated to the sur-  
157 face 0-2 cm soil moisture content (Njoku et al., 2003), while SMOS maps land soil moisture for  
158 the 0-5 cm depth. Level 3 CATDS (Centre Aval de Traitement des Donnees SMOS) products  
159 (Jacquette et al., 2010) are acquired. SMOS and AMSR-E are selected from ascending and  
160 descending passes, respectively, subject to their higher agreement to in-situ measurements (see,  
161 e.g., De Jeu and Owe, 2003; Draper et al., 2009; Jackson and Bindlish, 2012; Su et al., 2013).  
162 Both data products with a daily temporal resolution are spatially rescaled from  $0.25^\circ \times 0.25^\circ$  to  
163  $1^\circ \times 1^\circ$  resolution using the nearest neighbor interpolation to match W3RA. Note that these soil  
164 moisture observations are used in different periods during the assimilation process, i.e., AMSR-  
165 E soil moisture is assimilated for the period 2002-2011 and SMOS soil moisture is assimilated  
166 for the period 2011-2013.

### 167 2.2.3. Precipitation

168 Furthermore, monthly precipitation data of the Tropical Rainfall Measuring Mission  
169 Project (TRMM-3B43 products; version 7, TRMM, 2011; Huffman et al., 2012) are used to  
170 assess climate induced water storage changes. Due to the fact that ground validation over land is  
171 applied for TRMM-3B43 products, uncertainty in measured precipitation are smaller compared  
172 to those of the oceans. Several studies have implemented and validated these products over  
173 South America and proved their capabilities (see, e.g., Condom et al., 2011; Ceccherini et al.,  
174 2015; Cabrera et al., 2016). The rainfall data are provided on a  $0.25^\circ \times 0.25^\circ$  gridded spatial  
175 resolution and to make them comparable to those of the model (cf. Section 2.1), they are  
176 converted to  $1^\circ \times 1^\circ$  using the nearest neighbor interpolation for the period of 2002 to 2013.

### 177 2.3. Surface storage data

178 Although the focus of the present study is on sub-surface water storage compartments,  
179 in order to efficiently assimilate GRACE TWS data into W3RA, however, a special focus should  
180 be invested on surface water storage variations due to their large contribution in water storage  
181 changes over South America (Getirana et al., 2017). In particular, this is important because  
182 many surface water sources (in different forms, e.g., lakes and rivers, except for a few major  
183 ones) are not modeled in W3RA. To address this problem, the recently developed surface water  
184 storage data provided by Getirana et al. (2017) is used. The data is based on a coupled system  
185 compromising Noah land surface model (LSM) with multi-parameterization options (Noah-MP;  
186 Niu et al., 2011) and the Hydrological Modeling and Analysis Platform (HyMAP) river routing

187 scheme (Getirana et al., 2012). Multiple meteorological forcings and precipitation datasets are  
188 used to generate an ensemble of 12 runs, and to establish reference product with associated  
189 uncertainties (see details in Getirana et al., 2017). The  $1^\circ \times 1^\circ$  monthly gridded surface water  
190 data for the period of 2012 to 2013 are subtracted from GRACE TWS before data assimilation.

#### 191 2.4. In-situ groundwater measurements

192 In order to evaluate the obtained data assimilation results, independent in-situ ground-  
193 water measurements over 34 stations obtained from Global Groundwater Network (GGMN;  
194 <https://ggmn.un-igrac.org/>) and propagated within the study area (see Figure 1) are compared  
195 with estimated groundwater storage changes obtained from data assimilation. Groundwater  
196 level measurements should be converted into groundwater (GW) storage, which requires spe-  
197 cific yield values. In the absence of such information, following Tangdamrongsub et al. (2015),  
198 TWS variation from GRACE and Global Land Data Assimilation System (GLDAS, Rodell et  
199 al., 2004) soil moisture are used to calculate the specific yield and scale the observed head. The  
200 scaled in-situ groundwater level fluctuations are then used to assess the results. Afterwards, the  
201 assimilation results are spatially interpolated to the location of the in-situ measurements us-  
202 ing the nearest neighbor (the closest four grid values). The Root-Mean-Squared Error (RMSE)  
203 and correlations between the in-situ and estimated groundwater storage measurements are then  
204 computed.

#### 205 2.5. Data assimilation filtering method

206 The filtering technique of Ensemble Square-Root Filter (EnSRF) proposed by Whitaker  
207 and Hamill (2002) is used to assimilate GRACE TWS and soil moisture data into the W3RA  
208 model. The method is based on a traditional Ensemble Kalman Filter (EnKF) that poses a new  
209 sampling scheme. The filtering process starts with the forecast step, which includes integrating  
210  $N$  (ensemble number) samples of model state  $X$  that contains top soil, shallow soil, and deep  
211 soil water, snow, vegetation, and groundwater by a dynamical model. The forecast state, thus,  
212 can be shown as,

$$X^f = [X_1^f \dots X_N^f], X_i^f i = 1 \dots N, \quad (1)$$



213 where ‘f’ stands for forecast (‘a’ in following represents analysis). The corresponding model  
 214 state forecast error covariance of  $P^f$  and the mean state forecast  $\bar{X}^f$  are defined by:

$$P^f = \frac{1}{N-1} \sum_{i=1}^N (X_i^f - \bar{X}^f)(X_i^f - \bar{X}^f)^T, \quad (2)$$

$$\bar{X}^f = \frac{1}{N} \sum_{i=1}^N (X_i). \quad (3)$$

215 The update stage in EnSRF contains two steps. First, it updates the ensemble-mean following,

$$\bar{X}^a = \bar{X}^f + K(y - H\bar{X}^f), \quad i = 1 \dots N, \quad (4)$$

$$K = P^f(H)^T(HP^f(H)^T + R)^{-1}, \quad (5)$$

216 where  $K$  is the Kalman gain,  $y$  is the observation vector and transition matrix is indicated  
 217 by  $H$ .  $R$  represents the observation covariance matrix. Data assimilation methods are largely  
 218 sensitive to the observations uncertainties. Therefore, it is important to assign accurate error  
 219 values to each observation used in data assimilation. Here, for GRACE observations, TWS  
 220 error covariance matrix is constructed from Full error information about the GRACE Stokes’  
 221 coefficients. There is no covariance error information available for satellite soil moisture ob-  
 222 servations, thus, we assume their error covariances to be uncorrelated and consider various  
 223 uncertainties to monitor their impacts on data assimilation by comparing the results with inde-  
 224 pendent measurements. This allows us to obtain optimum error values for soil moisture part of  
 225 observation error covariance. Accordingly,  $\mathbf{R}$  is assumed to be diagonal with an error standard  
 226 deviation of  $0.04 (m^3m^{-3})$  for SMOS (suggested by Leroux et al., 2016) and  $0.05 (m^3m^{-3})$  for  
 227 AMSR-E (suggested by De Jeu et al., 2008). In addition, for the observation error covariance  
 228 in simultaneous data assimilation case, GRACE data and both SMOS and AMSR-E observa-  
 229 tions are assumed to be uncorrelated. It is worth mentioning that more study is still required  
 230 to efficiently estimate the spatially varying observations uncertainties, which also account for  
 231 error correlations. This can lead to different results and potentially improved data assimilation.  
 232  $\bar{X}^a$  in Equation 4 is the analysis ensemble-mean. In the next step, i.e., the analysis step, the

233 filter updates the forecast ensemble of anomalies,

$$A^f = [A_1^f \dots A_N^f], \quad (6)$$

$$A_i^f = X_i^f - \bar{X}^f, \quad (7)$$

234 into the analysis ensemble deviation  $A^a$  in Equation 8. EnSRF exploits the serial formulation  
 235 of the Kalman filter analysis step in which the observations are assimilated each at a time to  
 236 compute the analysis perturbations that exactly match the Kalman filter covariance (Hoteit et  
 237 al., 2008) using the modified gain ( $\tilde{K} = \alpha K$ ) with,

$$A^a = (I - \tilde{K}H)A_i^f, \quad (8)$$

$$\alpha = \left(1 + \sqrt{\frac{R}{HP^fH^T + R}}\right)^{-1}, \quad (9)$$

238 where  $I$  is an identity matrix. This definition requires the observation errors to be uncorre-  
 239 lated, which can always be satisfied by scaling the observations with the square-root inverse of  
 240 the observational error covariance matrix (Hoteit et al., 2015). This, however, is not the case  
 241 here because there is no rank deficiency on observation error covariance. We assume that soil  
 242 moisture observations are uncorrelated. Furthermore, the correlation between GRACE TWS  
 243 on the one hand and soil moisture observations, on the other hand, is also assumed to be zero.  
 244 The rank deficiency issue raised from GRACE TWS block in the covariance matrix is mitigated  
 245 by applying GRACE TWS observations in a  $3^\circ \times 3^\circ$  spatial resolution along with the implemen-  
 246 tation of Local Analysis (LA) (Evensen, 2003) scheme, which restricts the information used  
 247 for the covariance matrix computation to a spatially limited area and uses only measurements  
 248 located within a certain distance from a grid point (cf. Section 2.6, see also Khaki et al.,  
 249 2017b). More details regarding the EnSRF algorithm and its performance in GRACE TWS  
 250 data assimilation against other filters are described, e.g., in Whitaker and Hamill (2002) and  
 251 Khaki et al. (2017a).

## 252 2.6. Experimental setup

253 As already mentioned, the state vector includes different water storages, i.e., soil mois-  
 254 ture, vegetation, snow, and groundwater, simulated by W3RA. Previous studies have investi-  
 255 gated the surface water variations over South America (e.g., De Paiva et al., 2013; Getirana  
 256 et al., 2017), thus, we only focus on the estimation of sub-surface compartments; groundwater

257 and soil moisture. The modified GRACE TWS data (cf. 2.3) is then used to update the above  
258 water compartments excluding surface storage. The observation operator aggregates different  
259 water storages at each grid point (1688 points in total) to update with GRACE TWS and scales  
260 top-layer soil storage by the field capacity value to provide a relative wetness for updating with  
261 soil moisture products of AMSR-E and SMOS (Renzullo et al., 2014).

262 Considering the different temporal resolution of assimilation observations, e.g., monthly  
263 GRACE TWS and daily soil moisture measurements, both observation sets are temporally  
264 rescaled into a 5-day resolution for data assimilation. This is done to allow for a simultaneous  
265 data assimilation of GRACE TWS and satellite soil moisture measurements. Khaki et al.  
266 (2017b) showed that assimilating GRACE TWS in a 5-day temporal scale leads to a better  
267 improvement in state variables compared to daily and monthly scales. Therefore, in the analysis  
268 steps during the assimilation, the 5-day temporal average update increment (cf. Equation 4)  
269 is applied. In order to produce ensemble for EnSRF filtering, we use Monte Carlo sampling  
270 of multivariate normal distribution, with the errors representing the standard deviations to  
271 perturb three main forcing parameters; precipitation, temperature, and radiation (see details  
272 in Renzullo et al., 2014). Afterwards, by integrating perturbed meteorological forcing forward  
273 in time with the model from 2000 to 2002, 72 sets of state vectors (ensemble; as suggested by  
274 Oke et al., 2008) is created at the beginning of the study period.

275 While implementing data assimilation with a large number of ensemble members results  
276 in a heavy computational burden, using a small ensemble size can also be problematic, as  
277 it can lead to filter divergence or inaccurate estimation (Tippett et al., 2003). To address  
278 this issue, two filter tuning is applied including ensemble inflation and LA. Ensemble inflation  
279 helps ensemble members to adequately span the model sub-space by inflating prior ensemble  
280 deviation from the ensemble-mean and increases their variations (Anderson, 2001; Anderson et  
281 al., 2007). Various inflation factors ( $[1 - 1.8]$ ) are tested and their impacts ensemble spreads  
282 are monitored to determine the best value (i.e., 1.12). Furthermore, LA (Evensen, 2003; Ott et  
283 al., 2004) is applied to both account for a limited ensemble number and also GRACE limited  
284 spatial resolution. Applying GRACE TWS data on a high spatial resolution (e.g.,  $1^\circ \times 1^\circ$ ) causes  
285 correlation errors, which degrades the performance of data assimilation (Khaki et al., 2017a,b).  
286 Khaki et al. (2017b) showed that LA can successfully mitigate this problem by restricting the  
287 impact of the measurements in the update step to variables located within a certain distance  
288 only, e.g,  $5^\circ$ , which is applied in the present study.

289 *2.7. Climate variability impacts*

290 In order to investigate the model’s enhancement for studying climate induced impacts,  
 291 TRMM rainfall and ENSO data are employed. At each grid point, correlations between TWS  
 292 with and without data assimilation for both rainfall (at the same point) and ENSO are calcu-  
 293 lated. Afterwards, improvements achieved by data assimilation with respect to no assimilation  
 294 of TWS are explored. Furthermore, principal component analysis (PCA; Lorenz, 1956) is ap-  
 295 plied on the estimated groundwater and soil moisture storages (from assimilation), as well as  
 296 on TRMM rainfall to better analyze the spatio-temporal changes of water storages and pre-  
 297 cipitation. This is done to examine the precipitation patterns within the area between 2002  
 298 and 2013 and to investigate their connections to water storage changes. Since precipitation is  
 299 the major effective parameter on water storage recharge, the process helps to study the role  
 300 of climate variability on water storage variations. A schematic illustration of the methodology  
 301 steps is provided in Figure 2.

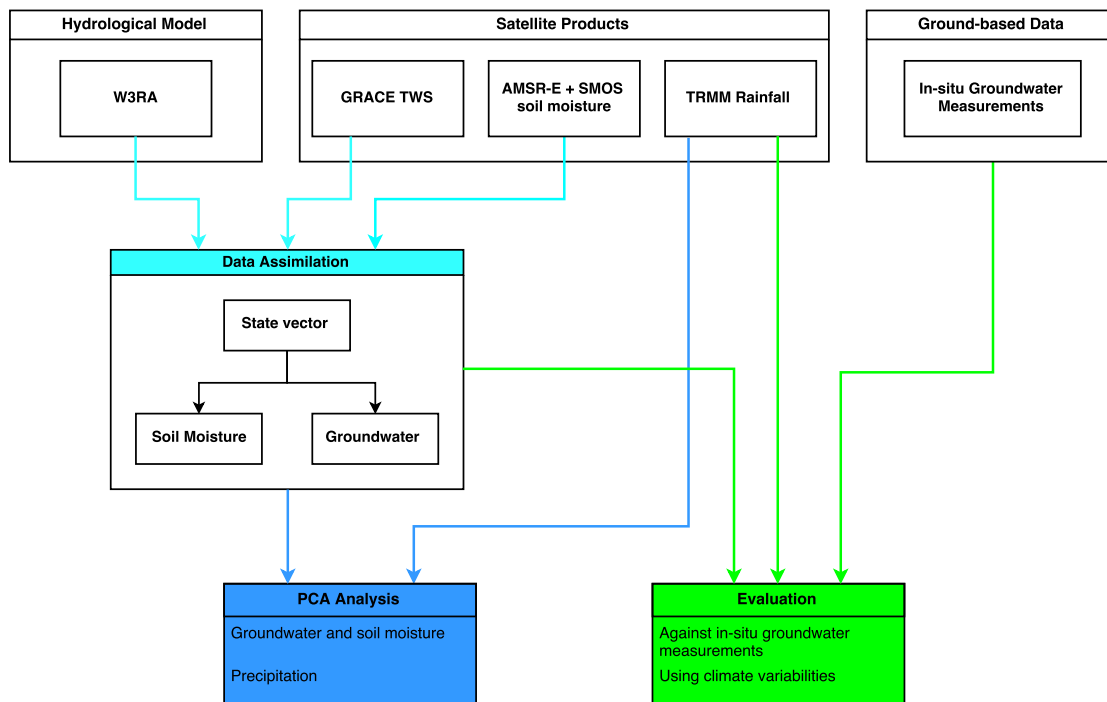


Figure 2: Schematic illustration of the methodology steps including data used, assimilation scheme, and evaluation processes. In data assimilation process, W3RA is used for forecasting and GRACE TWS and satellite soil moisture measurements are used to update forecasts from the model. Once the groundwater and soil moisture are estimated from the assimilation process, their relationship with rainfall data is investigated using PCA analysis. The in-situ groundwater measurements as well as rainfall data are further used to assess the data assimilation estimates.

## 302 **3. Results and discussions**

### 303 *3.1. Data assimilation*

304 In what follows, data assimilations results and their comparison with in-situ measure-  
305 ments are first discussed. First, we investigate the impacts of assimilated observations, e.g.,  
306 GRACE TWS and satellite soil moisture on water storage estimates (cf. Section 3.1.1). Note  
307 that the results presented in this section are not used for validation and only show how the  
308 assimilation results differ from the open-loop (no data assimilation) results. Evaluation against  
309 independent measurements will also be discussed (cf. Section 3.1.2).

#### 310 *3.1.1. Observation impacts on state variables*

311 The spatially averaged time series of TWS variations estimated by EnSRF over South  
312 America is presented in Figure 3a, which shows that the application of data assimilation re-  
313 duces misfits (Figure 3b) between the results and GRACE TWS compared to the open-loop.  
314 Furthermore, Figure 3c shows the average time series of soil moisture variations from the model  
315 top layer open-loop and assimilation, as well as satellite remote sensing. Similar to Figure  
316 3b, Figure 3d indicate that the data assimilation successfully decreases the differences between  
317 soil moisture estimates and the observations. The average discrepancy between the estimated  
318 (assimilated) TWS and those by GRACE is approximately 46%, and between soil moisture  
319 estimates and satellite (AMSR-E and SMOS) observations is 34% less than those of between  
320 open-loop and observations, which demonstrate that data assimilation successfully incorporates  
321 observations into the system states. The effects of data assimilation can better be seen where  
322 large anomalies exist such as 2005 and 2011. The large anomaly in Figure 3a during 2011 could  
323 be related to the strong ENSO impact (see, e.g., Boening et al., 2012). It is clear that this  
324 strong anomaly captured by GRACE is successfully reflected into assimilation TWS contrary  
325 to that of open-loop.

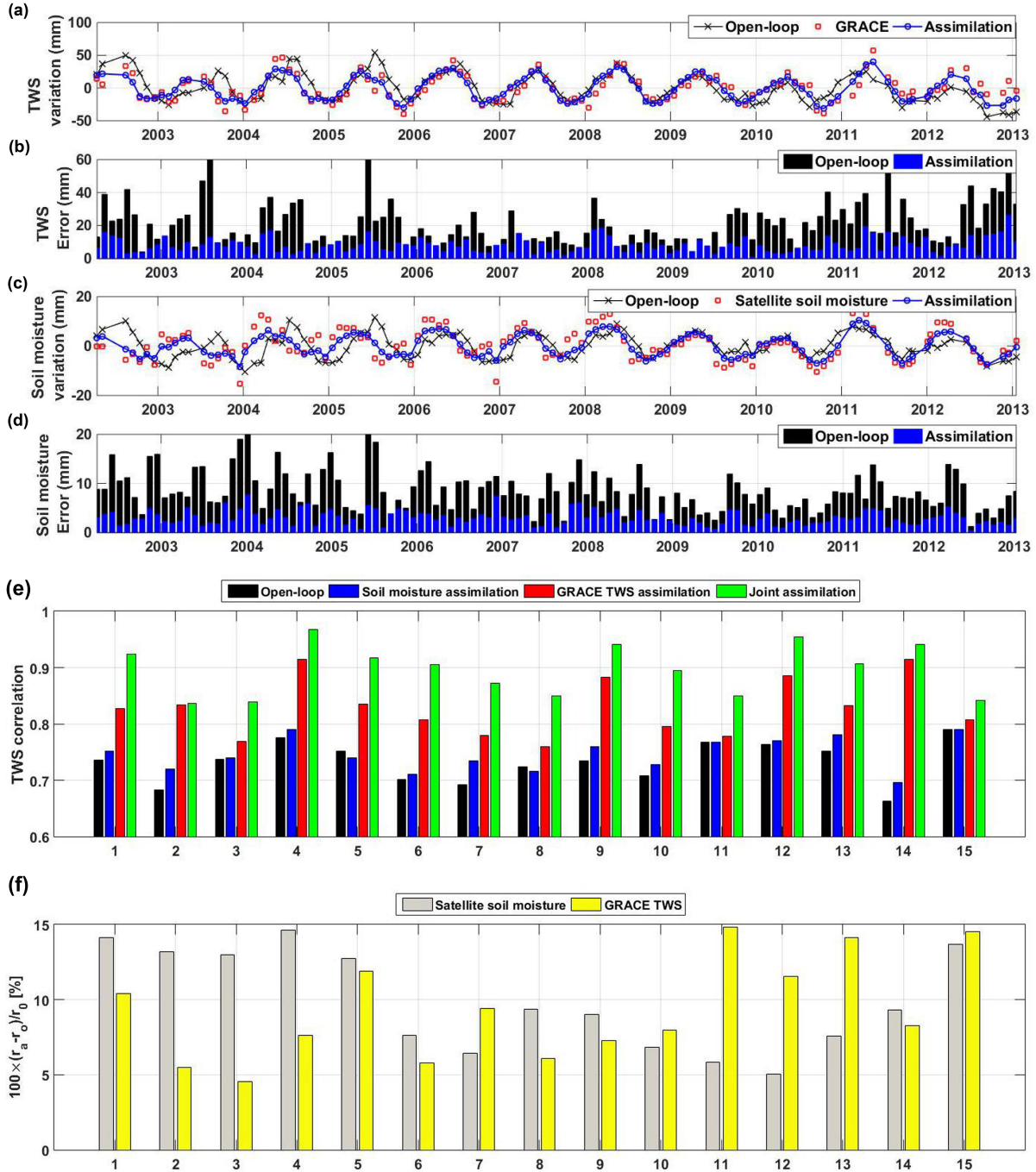


Figure 3: (a) Comparison between the TWS time series from the assimilation process (blue), GRACE TWS (red), with the open-loop referring to the model estimation without applying data assimilation (black). (b) Absolute error bars before (black) and after (blue) data assimilation process in comparison to the GRACE TWS observations. (c) and (d) are similar to (a) and (b), respectively, but for soil moisture observations. (e) Average correlations between GRACE-derived TWS and TWS simulated by W3RA before assimilation, GRACE TWS only assimilation, soil moisture only assimilation, and joint data assimilation for each basin (cf. Figure 1). (f) Correlation improvement between joint data assimilation results and GRACE TWS and soil moisture observation with respect to the open-loop results.

326 For a better discussion, we also calculate the correlation between the soil moisture variations  
327 from satellites and estimations for each of the 15 basins (Figure 3e). This is done on a basin  
328 scale due to the fact that basin averaged time series can be more representative of water stor-  
329 age changes in the area. In all the cases, regardless of the method, data assimilation resulted  
330 in higher correlations with the observations compared to the open-loop (un-assimilated model  
331 products). Assimilation of only one satellite products, e.g., GRACE TWS or soil moisture,  
332 increases the correlation values in Figure 3e. As expected, GRACE TWS data assimilation has  
333 more effects on enhancing TWS correlations, however, it can be seen that even soil moisture  
334 only data assimilation in most of the cases causes higher TWS correlation than the open-loop  
335 results. It can also be seen that the correlation between joint data assimilation (GRACE TWS  
336 and satellite soil moisture) results in Figure 3e are largely in agreement with the observed  
337 variables compared to GRACE-only data assimilation. This indicates that assimilation of soil  
338 moisture products along with GRACE TWS leads to more improvements. One main reason for  
339 this is that while GRACE TWS data assimilation is generally an effective approach for updating  
340 models TWS (e.g., Zaitchik et al., 2008; Reager et al., 2015; Khaki et al., 2018a,b), it can also  
341 introduce artifact effects to different storage such as by assigning wrong increments to either  
342 groundwater or soil moisture (Li et al., 2015; Giroto et al., 2017; Khaki et al., 2018c). Assim-  
343 ilation of soil moisture products can account for this problem by independently constraining  
344 soil moisture estimates. Figure 3e shows that this joint assimilation leads to better estimations  
345 of soil moisture.

346 In addition, the average correlation improvement from jointly assimilating GRACE TWS  
347 and soil moisture in comparison to the open-loop is presented in Figure 3f. Note that only the  
348 results of joint data assimilation are presented in the figure due to its better performance (cf.  
349 Figure 3e). Figure 3f demonstrates that higher correlations are achieved after data assimi-  
350 lation. For GRACE TWS, higher correlations are achieved within larger basins such as Amazon  
351 (number 15) and Tocantins (number 11). This suggests that GRACE TWS data assimilation  
352 has larger impacts on these basins. It can be seen that the minimum improvement happens  
353 for the Pacific Coast, North Chile basin (number 3), where GRACE TWS data are expected  
354 to have larger errors in comparison to other basins like the Amazon basin with small leakage  
355 errors (Wiese, 2015). Nevertheless, in general, the assimilation process increases the correlation  
356 between outputs and GRACE TWS.

357 *3.1.2. Evaluation results*

358 In order to examine the validity of the data assimilation, groundwater in-situ measure-  
 359 ments from various stations are spatially averaged to the location of nearest model grid points  
 360 and compared with their estimates. As mentioned (cf. Section 2.4), we calculate RMSE and  
 361 correlation for three tests including the open-loop, GRACE-only TWS data assimilation, and  
 362 joint GRACE-soil moisture assimilation. Table 1 presents the average RMSE, corresponding  
 363 RMSE reduction, and Nash-Sutcliffe coefficient (NSE) of the results before and after assimila-  
 364 tion. In order to statistically assess the significance of the results, the student t-test is applied  
 365 after considering the autocorrelation in time series. The estimated t-values and the distribu-  
 366 tion at 0.05 significant level are used to calculate p-values. Data assimilation results indicate  
 367 significantly smaller RMSE and higher NSE in cases of GRACE TWS and joint data assimi-  
 368 lation. Soil moisture only data assimilation has small positive impacts on NSE improvement  
 369 (e.g., 3%) but with no significant RMSE improvement. An average improvement of 23.43%  
 370 in RMSE and 14.08% in NSE (for all assimilation experiments) proves the capability of data  
 371 assimilation to improve model simulations with respect to the reality. Nevertheless, the joint  
 372 data assimilation indicates larger improvements in terms of RMSE reduction and NSE improve-  
 373 ments than GRACE-only data assimilation. This shows that this method can better constrain  
 374 different water storage compartments. It can be seen that soil moisture observations help in  
 375 better controlling the distribution of increments between storages.

Table 1: Statistics of groundwater errors. For each case, the RMSE average and its range ( $\pm XX$ ) at the 95% confidence interval is presented. Improvements in data assimilation results are calculated with respect to the groundwater storages from the model without implementing data assimilation.

Experiment scenario	NSE	RMSE (mm)	Improvement (%)	
			NSE	RMSE
Open-loop	0.63	69.26 $\pm$ 7.38	–	–
GRACE-only data assimilation	0.75	54.19 $\pm$ 5.79	16.01	21.76
Soil moisture data assimilation	0.65	66.48 $\pm$ 7.12	3.07	–
Joint GRACE-soil moisture assimilation	0.82	51.87 $\pm$ 5.16	23.17	25.11

376 Furthermore, it is found that this joint data assimilation better reduces the forecast un-  
 377 certainties. We calculate the average standard deviation (STD) of ensemble members before  
 378 and after each data assimilation step for all assimilation cases. These ensemble uncertainties



379 generally refer to forcing errors that grow by running the model forward in time. While all  
380 the cases, as expected, lead to a smaller STD (5.31% on average) in the analysis steps (af-  
381 ter assimilating observations), the least uncertainty is achieved for the joint data assimilation  
382 (11.78% STD reduction). Note that the smaller ensemble STD can also lead to a weaker en-  
383 semble spread, however, this is not the case here. The achieved STD reduction means that the  
384 method can better propagate ensemble members by improving the spread of forecast ensemble  
385 members based on the observations and their associated uncertainties. These results show that  
386 data assimilation can improve our understanding of water storage changes. More importantly,  
387 monitoring groundwater using reliable information is crucial over South America, where only  
388 a few studies have focused on it (e.g., [International Groundwater Resources Assessment Cen-  
389 tre, 2004](#); [Villar, 2016](#)). Groundwater is a major water resource along with surface storages  
390 within the area providing almost 60% of freshwater use ([Villar, 2016](#)). This number is even  
391 higher for some countries such as Chile, Peru, Venezuela, Suriname and The Guyanas ([Morris  
392 et al., 2003](#)). The application of the proposed approach for studying groundwater variations can  
393 benefit many of these countries to better monitor groundwater using the enhanced estimates.

394 As previously mentioned, data assimilation, especially when using GRACE TWS data, can  
395 introduce artifacts to other variables. This can be the case not only for different variables in  
396 the state vector (e.g., groundwater and soil moisture) but also for non-assimilated variables  
397 such as water discharge. To monitor this effect, we compare model water discharge to stream-  
398 flow in-situ measurements obtained from Hydrology and Geochemistry of the Amazon basin  
399 (HYBAM). The monthly in-situ discharge measurements, computed as the sum of the daily  
400 discharge, are spatially interpolated to the closest grid points and compared with the estimates  
401 at those grid points. Figure 4a shows the average discharge time series over the Amazon basin  
402 before and after data assimilation, as well as from in-situ measurements. It can be seen that  
403 assimilation of GRACE TWS and soil moisture reduces the misfits between model and in-situ  
404 water discharge time series. Furthermore, Figures 4b and 4c present the average scatter plots  
405 of the discharge estimates from the open-loop and assimilation compared to the in-situ values.  
406 The average correlations between time series are also indicated in the plots, which show the  
407 larger agreement between the assimilation results and in-situ streamflow measurements. Data  
408 assimilation decreases the RMSE values from 6.47 cm to 2.88 cm and increases NSE from 0.47  
409 to 0.71. Assimilation of GRACE TWS and soil moisture, thus, effectively reduces discharge  
410 error. This confirms the findings of [Syed et al. \(2005\)](#), who used GRACE TWS and additional

411 model-derived fluxes observations to study water discharge over the Amazon basin. Under-  
 412 mining groundwater and moisture storage changes in their experiment, however, led to some  
 413 degree of discrepancy between the estimated and observed discharge. In contrast, in this study,  
 414 updating different water compartments including groundwater during the assimilation analysis  
 415 results in a better agreement between the results and in-situ measurements. In general, Figure 4  
 416 indicates that the joint assimilation process not only causes any artifact errors but also improve  
 417 the discharge estimates (cf. Figure 4).

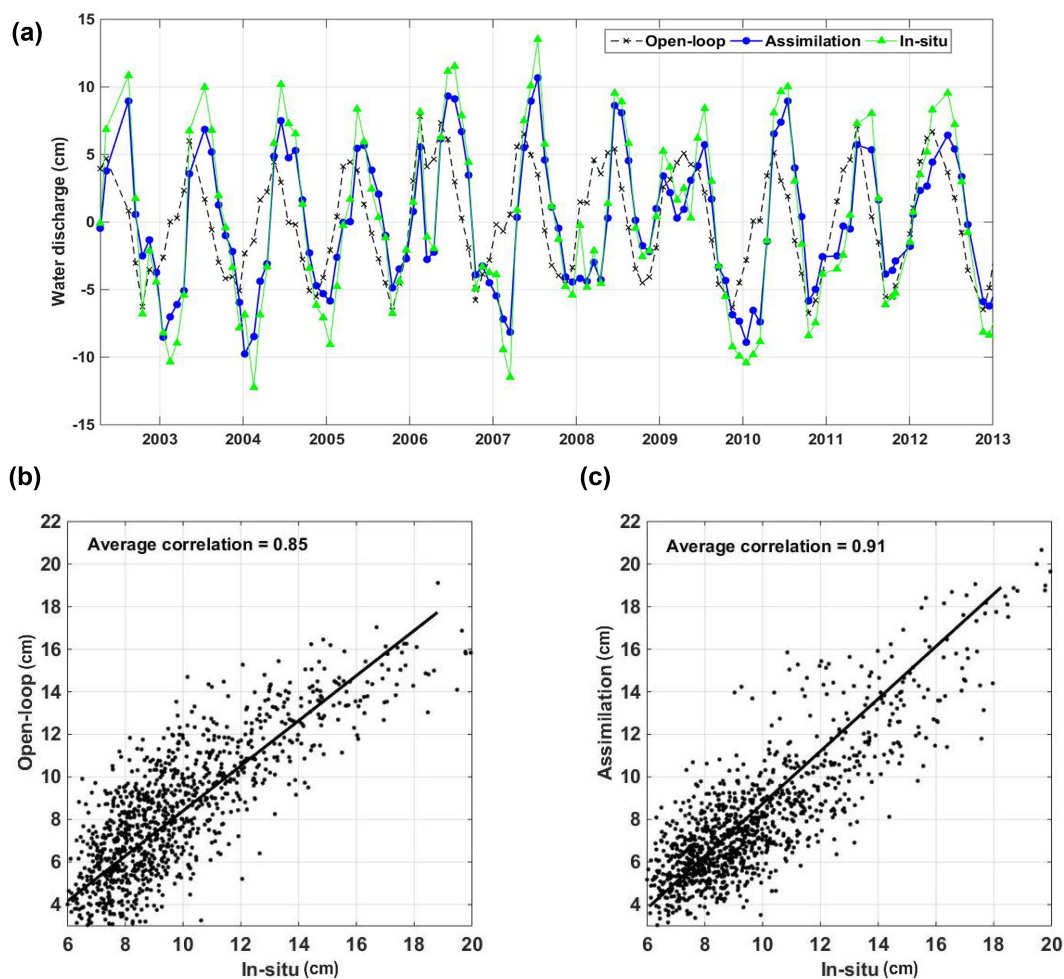


Figure 4: (a) Average discharge time series before and after data assimilation, as well as from in-situ measurements. Scatter plots of average discharge from the open-loop and joint data assimilation with respect to in-situ measurements are presented in (b) and (c), respectively.

418 To further investigate the effect of data assimilation, we compare the TWS estimates from  
 419 the joint data assimilation and the open-loop run with precipitation over the Amazon Basin.

420 The rationale behind this choice is due to the fact that various studies have reported different  
 421 droughts (see, e.g., [Chen et al., 2009](#); [Frappart et al., 2013](#)) over the basin and a successful data  
 422 assimilation should be able to capture these phenomena. Figure 5 shows the TWS variations  
 423 over the basin from the above approaches, as well as precipitation. The average correlation  
 424 between TWS estimates and precipitation is 0.89,  $\sim 17\%$  larger than that of the open-loop run.  
 425 It can be seen that the data assimilation time series better capture large anomalies such as in  
 426 2004 and 2009 reflected also in the precipitation time series. La Niña impact during 2011 (see  
 427 also [Boening et al., 2012](#)) is better captured by the assimilation results. Furthermore, 2005  
 428 drought over the Amazon Basin (see, e.g., [Chen et al., 2009](#)) is reflected in both open-loop and  
 429 assimilation results, while the later show a larger amplitude.

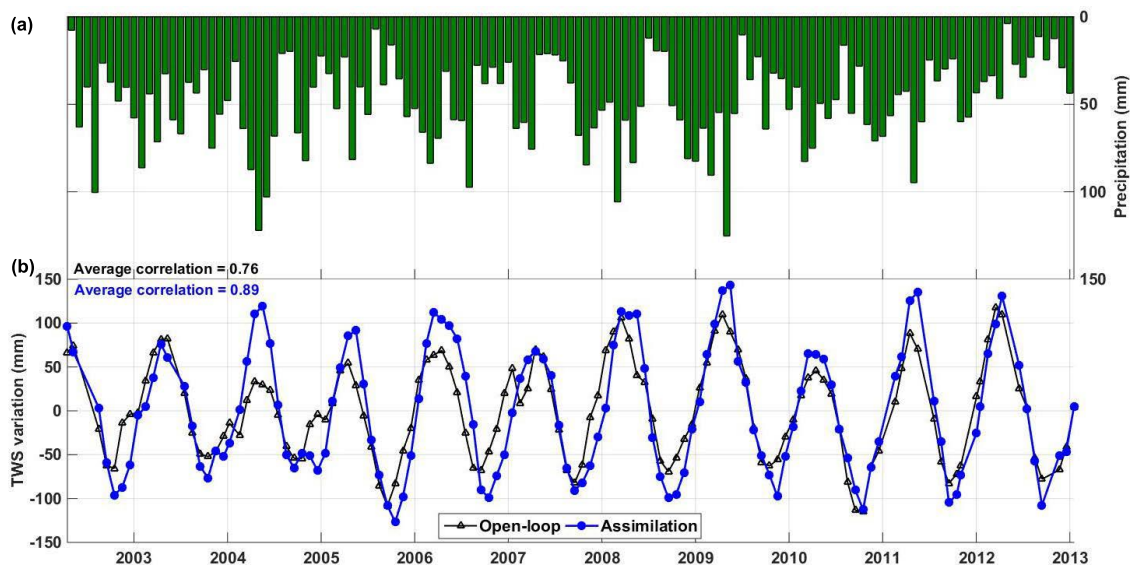


Figure 5: Average precipitation (a) and TWS time series from the open-loop and joint data assimilation (b) over Amazon basin.

430 Table 2 contains the correlations between the open-loop run and joint data assimilation  
 431 TWS results and precipitation. The table also reports the correlation improvements in the  
 432 assimilation results with respect to those of the open-loop against both precipitation as well  
 433 as ENSO (using Niño 3.4 indicator), as the dominant climate variability index over South  
 434 America ([Tourre et al., 2008](#); [Xavier et al., 2010](#); [Flantua et al., 2016](#)) for each basin. It can be  
 435 seen that significant improvements are achieved by assimilating remotely sensed TWS and soil  
 436 moisture observations into W3RA hydrological model. Correlation with both precipitation and

437 ENSO over a majority of the basins showcase these improvements. Note that only precipitation  
438 correlation improvements are statistically significant. An average correlation between rainfall  
439 and TWS anomalies within South America is found to be 0.89,  $\sim 11\%$  larger than the open-  
440 loop results. This indicates that there is a larger agreement between the assimilation results  
441 and rainfall over the area than the case of the model simulations without data assimilation.  
442 The improvements in terms of correlations with ENSO are different for various basins. For  
443 example, larger correlations and corresponding improvements are estimated for Atlantic North  
444 Coast (basin 5), Pacific Coast, North Chile (basin 3), Negro (basin 10), Magdalena (basin 4),  
445 and Orinoco (basin 12) basins. The reason for this is due to the fact that ENSO effects on  
446 precipitation are larger over basins located within the north towards the northeast and the  
447 southeast parts of South America and partially over the Amazon basin (Flantua et al., 2016).  
448 These larger effects lead to a similar impact on water storage changes that is successfully  
449 captured by data assimilation results. In general, larger correlations between the estimated  
450 TWS and precipitation over larger basins, e.g., Amazon (basin 15), La Plata (basin 14), and  
451 Sao Francisco (basin 13) are also found. This could be due to the ability of GRACE to solve  
452 larger basins that better constrain system states during data assimilation.

Table 2: Average correlation between the open-loop and assimilation TWS and precipitation. Correlation improvements are calculated using the increase of correlation between TWS from data assimilation and both precipitation and ENSO with respect to open-loop TWS.

Basins	Correlation to precipitation		Correlation improvements	
	Open-loop	assimilation	Precipitation	ENSO
(1) South-east Atlantic	0.88	0.90	2.27	3.33
(2) Pacific Coast, Peru	0.84	0.89	5.95	7.78
(3) Pacific Coast, North Chile	0.79	0.91	15.19	8.17
(4) Magdalena	0.87	0.92	5.75	7.23
(5) Atlantic North Coast	0.91	0.95	4.39	8.45
(6) Pacific Coast, South Chile	0.84	0.89	5.95	3.12
(7) Colorado Basin	0.78	0.91	16.67	1.72
(8) Atlantic South Coast	0.80	0.87	8.75	2.60
(9) North-east Atlantic	0.85	0.88	3.53	–
(10) Negro Basin	0.67	0.83	23.88	11.35
(11) Tocantins	0.69	0.89	28.98	4.54
(12) Orinoco	0.73	0.86	17.81	9.85
(13) Sao Francisco	0.92	0.92	–	3.06
(14) La Plata	0.75	0.94	25.33	5.17
(15) Amazon Basin	0.92	0.94	2.17	5.35

### 453 3.2. Water storage changes and climatic impacts

454 Average monthly TWS variations over South America from joint data assimilation is  
455 shown in Figure 6. Different time spans are used for the averaging period including 2003-2012  
456 (the entire study period) and 2005, 2009, 2010, 2011, and 2012 with remarkable extreme climate  
457 event that could potentially affect TWS anomalies. Larger water storage changes can be seen  
458 generally for basins located in the northern (e.g, Amazon basin) and southern (e.g., Orinoco  
459 and Negro basins) parts of South America. Figure 6 suggests that more water content, and  
460 subsequently more TWS variations exist over these areas. This could be due to the abundance of  
461 precipitation over these regions (see, e.g., [Sanso and Guenni, 1999](#); [Marengo, 2009](#); [Buytaert et al., 2013](#)).  
462 On the other hand, basins located in the west and northwest parts, e.g., Magdalena,  
463 Pacific Coast-Peru, and Pacific Coast-north Chile basins experience smaller TWS anomalies.  
464 The negative water storage anomalies in the northern parts (e.g., Amazon basin) of South  
465 America are observed during 2005 and 2010, and also in the southern parts (e.g., Negro basin)  
466 during 2009, 2010, 2011, and 2012. These results are supported by the findings of [Humphrey et al. \(2016\)](#)  
467 who also demonstrated water storage deficits, e.g., over northern parts (2004-2005),  
468 majority parts of Amazon basin (2010), and the western parts of South America (2011). The  
469 impact of the 2012 drought, which can be attributed to the anomalous SST in the Atlantic  
470 Ocean ([Pereira et al., 2014](#)) can clearly be seen within the eastern and southern parts of South  
471 America (see also [Sun et al., 2016](#)). Furthermore, El Niño effect in 2009 ([Tedeschi et al., 2013](#))  
472 and La Niña effect in 2011 ([Boening et al., 2012](#)) can be seen through large anomalies, e.g., in  
473 the north, northeast, and southern parts.

474 To better analyze spatio-temporal variations of sub-surface water storages within South  
475 America, PCA is applied to groundwater and soil moisture results. Figure 7 shows the first  
476 three dominant modes. Furthermore, rainfall variations both spatially and temporally are in-  
477 vestigated to explore their connections to water storage variations. Major water storages can be  
478 found from central to northern parts of South America, areas with rainfall patterns dominated  
479 by ENSO phenomena ([Carrillo et al., 2010](#)). This shows a larger amount of storages over the  
480 area mainly due to more rainfall. Considerable soil moisture content variations are found over  
481 North-east Atlantic (mode 2 and mode 3) and La Plata (mode 3). Larger groundwater varia-  
482 tions can also be seen in Amazon and La Plata. To a lesser degree, the Orinoco and Atlantic  
483 North Coast basins contain large signal variations both for groundwater and soil moisture. It  
484 can also be seen that both groundwater and soil moisture variations modestly follow the same

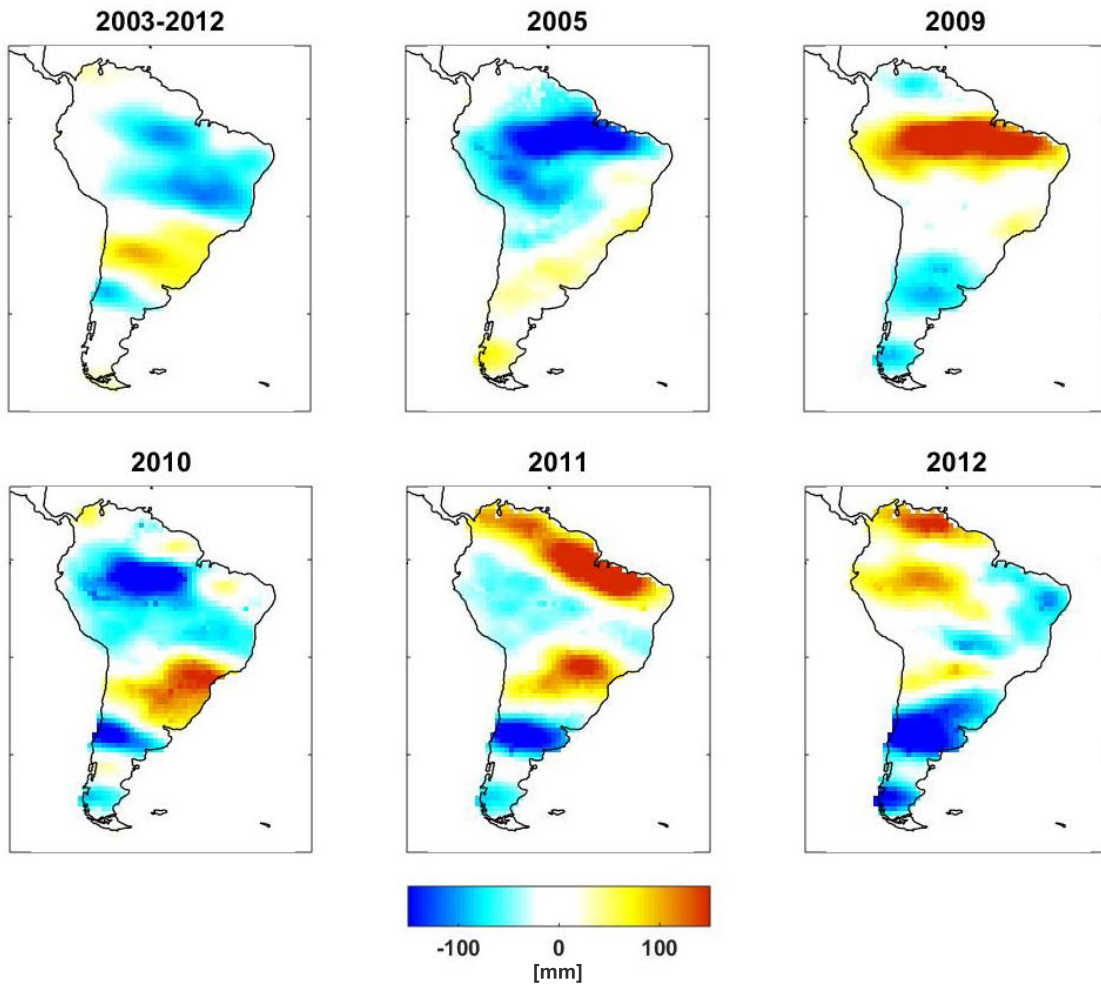


Figure 6: Average monthly TWS variations from data assimilation for different time periods.

485 pattern except for mode 3, where negative variations exist in the soil moisture map over the  
 486 south-eastern parts while the negative variations in groundwater map can be found over the  
 487 central to northern parts. The positive anomalies over northern parts in soil moisture vari-  
 488 ations, as it will be shown, matches precipitation patterns in the same areas. This suggests  
 489 that between the two water compartments, soil moisture variations follow precipitation more  
 490 closely, whereas groundwater changes which can largely be affected by non-climatic factors, e.g.,  
 491 anthropogenic impacts. In general, based on these maps, more sub-surface water variabilities  
 492 exist over the central towards northern and western parts of the continent compared to the  
 493 south-western areas.

494 In terms of temporal variations, the first three extracted principal components (PC) of



495 groundwater and soil moisture are also demonstrated in Figure 7. The time series of both  
496 water storages largely depict annual effects dominant over the majority of South America's  
497 parts including its central to the north. These parts are also affected by the Strong influence of  
498 La Niña for 2010-2011, as well as El Niño effect in 2008-2009. Negative trends in groundwater  
499 are captured by PC2 over the northeast and central toward western parts before 2006, between  
500 2007 and 2009, and also between 2010 and 2012. Such trends cannot be seen in soil moisture time  
501 series suggesting that non-climatic impacts such as the water used for power generation in Brazil  
502 (Sun et al., 2016) could possibly be responsible for the groundwater depletion. The negative  
503 soil moisture variations (mode 2) in the central part can be attributed to the multiple drought  
504 conditions, e.g., in the La Plata basin (2008-2009, Abelen et al., 2015). This soil moisture  
505 reduction was also reported by Escobar (2015) over the Amazon basin, which could be due to  
506 the anthropogenic impact on forest conservation. Dry events from 2012 to 2014 suggested by  
507 Humphrey et al. (2016) and Getirana (2016) can be seen in the northern and eastern parts of the  
508 South America, also reflected in groundwater and soil moisture time series (PC3 in Figure 7).  
509 Considerable anomalies are found in 2006-2007 and 2010 from groundwater and soil moisture  
510 mostly over the northern and eastern parts, which could be attributed to extreme climatic  
511 events in the same periods. On the other hand, a negative anomaly is detected in 2004 by both  
512 water storages. The 2005 dry condition effects on soil moisture is captured by soil moisture's  
513 second mode, which confirms the same impacts presented in Figure 6. The third mode of soil  
514 moisture time series depicts a negative anomaly for the period of 2002-2006 mostly over Negro  
515 basin, which, as will be shown, matches the third precipitation mode. El Niño effect in 2009  
516 causes groundwater negative anomaly in both modes 2 and 3 (see also Figure 6) affecting the  
517 central and eastern parts. Similar negative anomalies can also be seen in 2006 for groundwater,  
518 and in 2005 for soil moisture. A big part of these variations (e.g., over 2005, 2009-2012) can be  
519 related to climate variabilities while some of them, e.g., groundwater negative trends between  
520 2003 and 2006 and also 2007 and 2009, can be due to non-climate factors such as human usage  
521 and irrigations.

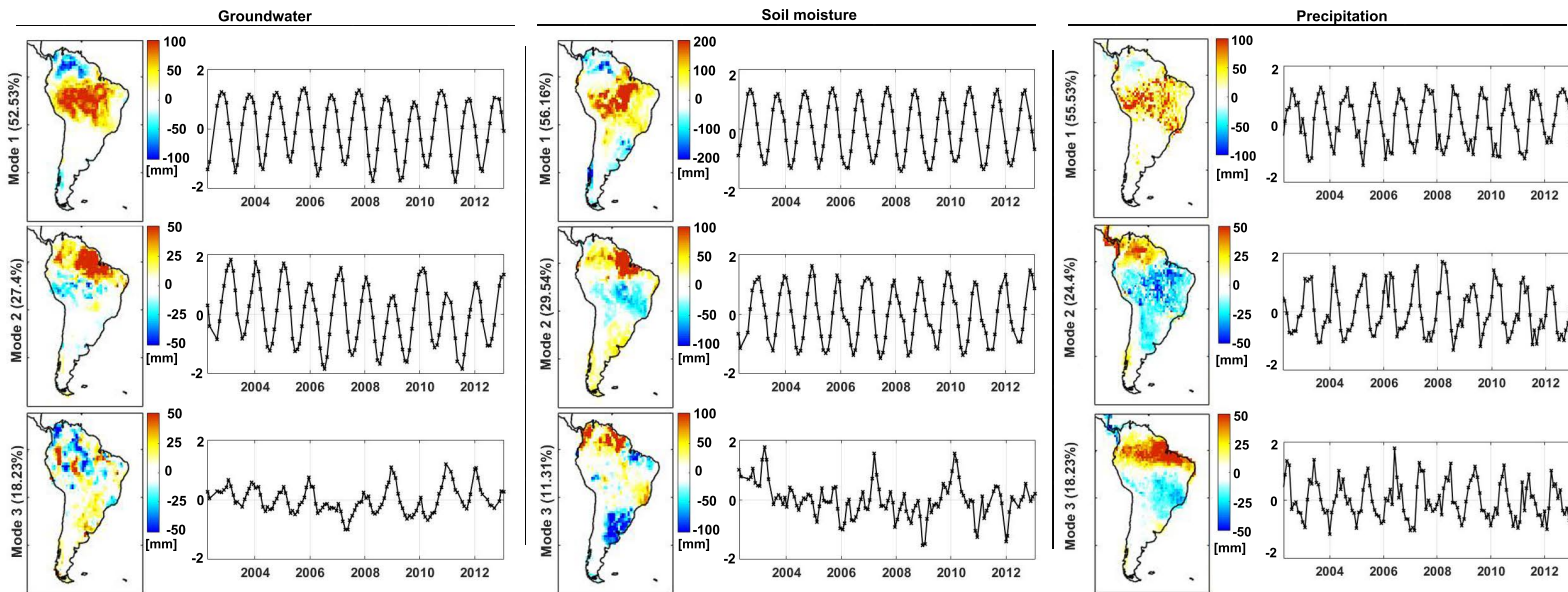


Figure 7: Three first modes of spatial distribution and temporal variations from the application of PCA on groundwater, soil moisture, and precipitation.

522 A major rainfall pattern is found over the central toward northern parts of South America,  
523 especially Amazon basin, where most of groundwater and soil moisture variations are explored.  
524 While the spatiotemporal distributions of rainfall are highly matched to those of groundwater  
525 and soil moisture in the first mode, the precipitation second mode is more correlated to that  
526 of soil moisture. This, as expected, indicates that precipitation has larger influence on soil  
527 moisture variations while groundwater can be largely affected by other factors (e.g., water  
528 usages). Next, Atlantic North Coast, La Plata, and Negro basins indicate larger signals in  
529 contrast to south-western basins, e.g., Pacific Coast, South Chile and Atlantic South Coast.  
530 Similar to groundwater and soil moisture mode 1, rainfall time series in Figure 7 also displays  
531 strong seasonal variations. In contrast to the negative anomalies in groundwater second mode  
532 time series, precipitation mode 2 does not show similar trends. However, both modes 2 and 3  
533 indicate a rainfall decline after 2012 mostly affecting the eastern toward northern parts (see,  
534 e.g., [Humphrey et al., 2016](#); [Getirana, 2016](#)). Similar to water storage time series, the La Niña  
535 effect can be observed for 2010–2011 ([Boening et al., 2012](#)). Large anomalies are also captured  
536 in 2005, 2006, and 2010, which considerably impacts water storages. El Niño effect in 2009 can  
537 also be seen in the second mode, which also affected groundwater and soil moisture variations  
538 within the central and south-eastern parts. A negative anomaly can be seen before 2004 in the



539 mode 3, which can be related to a weak El Niño causing negative anomalies of precipitation  
540 during the wet season (Juarez et al., 2009). Sun et al. (2016) suggested that this period exhibits  
541 months drier than the normal seasonal cycle of TWS due to the rainfall rates lower than the  
542 average. These prolonged reductions in rainfall can explain similar negative anomalies that  
543 occurred in groundwater and soil moisture time series seen.

544 Average trends for groundwater and soil moisture from the open-loop run and joint assimilation  
545 are presented in Table 3 for the basins. To this end, the modified Mann–Kendall trend  
546 test (Yue and Wang, 2002) is applied on deseasonalized time series. Note that the autocorrelation  
547 analysis is also used to compute an effective sample size and to correct the Mann–Kendall  
548 statistic. The trends when the p-values fall below 0.05 are considered statistically significant.  
549 It is worth mentioning that in addition to groundwater and soil moisture, the basin averaged  
550 precipitation time series are also considered here to investigate the climatic impacts on water  
551 storage changes. It can be seen that the application of data assimilation in many cases causes  
552 changes in either amplitude of trends or their signs. For example, over the Orinoco, the signs of  
553 variations become negative after data assimilation while these remained the same for La Plata  
554 with different amplitudes. For some other basins like South-east Atlantic, the trend values are  
555 close before and after data assimilation, which could be due to the smaller impacts of data  
556 assimilation.

557 It is also evident that there are larger agreements between precipitation and soil moisture  
558 trends. This further indicates that soil moisture changes mostly rely on rainfall pattern within  
559 South America. The mismatch between precipitation and groundwater trend signs over most of  
560 the basins, e.g., Pacific Coast, South Chile, Orinoco, South-east Atlantic and Colorado, suggests  
561 that non-climatic factors mostly influence the groundwater changes. This, in all of the cases,  
562 leads to a groundwater depletion while precipitation shows neither negative nor statistically  
563 significant trends. Nevertheless, negative trends are found in precipitation, soil moisture, and  
564 also groundwater over La Plata, Atlantic North Coast, Atlantic South Coast, and North-East  
565 Atlantic. Even though one can conclude that a majority of groundwater depletion over these  
566 basins can be caused by the precipitation decline, human impacts can still be an effective factor  
567 whereas assessing their contributions require additional information.

568 From Table 3, negative groundwater trends can be seen in most of the basins. For example,  
569 Sao Francisco and North-east Atlantic basins show the largest groundwater depletion compared  
570 to the other basins. This can be attributed to the fact that these basins have been under an

Table 3: Statistics of groundwater and soil moisture variation rates (mm/year) from the open-loop run and joint data assimilation. The statistically significant values at 95% confidence limit are demonstrated in bold.

Basins	Open-loop		Assimilation		Precipitation
	Groundwater	Soil moisture	Groundwater	Soil moisture	
(1) South-east Atlantic	<b>-0.37</b>	<b>-0.44</b>	<b>-0.57</b>	<b>+0.44</b>	<b>+0.09</b>
(2) Pacific Coast, Peru	<b>-0.10</b>	<b>-0.13</b>	<b>-1.09</b>	+0.12	+0.06
(3) Pacific Coast, North Chile	-	-	-0.03	-0.05	+0.13
(4) Magdalena	-0.02	<b>+0.16</b>	<b>+0.62</b>	+0.05	-0.01
(5) Atlantic North Coast	+0.02	+0.01	<b>-0.17</b>	<b>-0.23</b>	<b>-0.22</b>
(6) Pacific Coast, South Chile	-	-0.07	<b>-1.52</b>	<b>-0.76</b>	<b>+0.22</b>
(7) Colorado Basin	<b>-0.25</b>	<b>+0.20</b>	<b>-0.21</b>	<b>+0.23</b>	<b>+0.28</b>
(8) Atlantic South Coast	-0.06	-	<b>-0.57</b>	<b>-0.27</b>	<b>-0.12</b>
(9) North-east Atlantic	<b>+0.26</b>	+0.36	<b>-0.98</b>	<b>-0.47</b>	<b>-0.17</b>
(10) Negro Basin	-0.04	-	<b>-0.21</b>	-	-
(11) Tocantins	+0.02	+0.07	<b>+0.54</b>	+0.03	+0.02
(12) Orinoco	<b>+0.17</b>	<b>+0.35</b>	<b>-0.53</b>	+0.09	+0.01
(13) Sao Francisco	-0.07	-0.06	<b>-0.47</b>	<b>-0.24</b>	-0.03
(14) La Plata	<b>-0.89</b>	<b>+0.09</b>	<b>-1.09</b>	<b>-0.14</b>	<b>-0.10</b>
(15) Amazon Basin	+0.05	<b>+0.14</b>	+0.07	-0.02	+0.05

571 unprecedented water depletion as can be inferred from the studies of [Getirana \(2016\)](#) and [Sun et](#)  
572 [al. \(2016\)](#). Trend signs of soil moisture changes generally follow precipitation's. This, however,  
573 is different for some basins such as Pacific Coast, South Chile and Amazon. This mismatch  
574 over the Amazon basin can be explained by the fact that anthropogenic impacts on forest  
575 conservation results in soil moisture decline (see, e.g., [Escobar, 2015](#)). Similar negative trends  
576 are observed for both groundwater and soil moisture over La Plata, and also groundwater over  
577 Orinoco ([Ramirez et al., 2017](#)), which can be attributed to deforestation and excessive water  
578 use that have also been reported, e.g., by [Pereira et al. \(2011\)](#) for La Plata and [Ramirez et al.](#)  
579 [\(2017\)](#) for Orinoco basins (see also [Frappart et al., 2015](#)). There are also discrepancies between  
580 soil moisture and groundwater trend signs, e.g., over La Plata and Pacific Coast, North Chile.  
581 While the rate of the changes are smaller over Pacific Coast North Chile, La Plata, which are  
582 located in the most populated areas of South America, they have larger negative groundwater  
583 trends that could possibly be due to increased agricultural and livestock water usage in the basin  
584 (see also [Chen et al., 2010](#)). For some of the basins (e.g., the Amazon basin), the trends are  
585 not significant, especially the soil moisture and precipitation changes (e.g., over the Tocantins).  
586 In general, the annual rate of groundwater anomaly is -0.24 (mm/year) in South America,  
587 suggesting its depletion between 2002 and 2013. This could be due to climatic impacts (e.g.,  
588 droughts, see, e.g., [Bates et al., 2008](#); [Chen et al., 2010](#); [Treidel et al., 2011](#); [Getirana, 2016](#); [Sun](#)  
589 [et al., 2016](#)) and/or exponential increase of agriculture and industrial activities ([Bocanegra et](#)  
590 [al., 2010](#)). This negative trend is very important due to its effects on South America's water and

591 its use for agriculture. Groundwater is a major source of irrigation over most of the countries  
592 within South America such as major rice-growing regions of North Eastern Argentina, South  
593 Brazil and Uruguay (Herring, 2012). Besides, groundwater depletion can largely increase water  
594 quality challenges (e.g., Arsenic growth) as a potential issue over South America (see, e.g.,  
595 Munoz et al., 2002; Perez-Carrera and Cirelli, 2009; Herring, 2012).

#### 596 4. Conclusion

597 Multimission satellite datasets including Terrestrial water storages (TWS) from the  
598 Gravity Recovery And Climate Experiment (GRACE) satellite mission and soil moisture prod-  
599 ucts from the Advanced Microwave Scanning Radiometer - Earth Observing System (AMSR-E)  
600 and Soil Moisture and Ocean Salinity (SMOS) are assimilated into the World-Wide Water Re-  
601 sources Assessment (W3RA) model using the Ensemble Square-Root Filter (EnSRF) to increase  
602 the model performance for estimating groundwater and soil moisture over South America. The  
603 application of joint data assimilation causes improvements in W3RA estimates against ground-  
604 water in-situ measurements. This effect could clearly be seen for TWS estimates and impor-  
605 tantly for groundwater simulations, which emphasize the potentials of assimilating remotely  
606 sensed products to increase the reliability of the W3RA hydrological model. We further inves-  
607 tigate the correlation between assimilation results and precipitation from the Tropical Rainfall  
608 Measuring Mission (TRMM), as well as El Niño/Southern Oscillation (ENSO). The results  
609 indicate that assimilation TWS are more correlated to the TRMM rainfall and ENSO data  
610 compared to open-loop TWS estimates. Both of these assessments demonstrate the capability  
611 of data assimilation for improving model simulations of water resources over South America.  
612 Based on the results, the new information of groundwater and soil moisture are more reliable,  
613 which can be used for water management and agriculture objectives. From the application of  
614 principal component analysis (PCA) on water storage variations within South America and  
615 its 15 major basins, more soil moisture and groundwater anomalies are found over central to-  
616 ward northern and western parts of South America. Based on the results, a negative trend  
617 for groundwater is observed over most parts of South America. Negative trends are found for  
618 groundwater and to a lesser degree for soil moisture variations over the majority of the studied  
619 basins. This study shows that application of data assimilation can successfully improve our  
620 understanding of water storage changes. Nevertheless, more investigations are still needed to  
621 fully assess the approach's performance, e.g., by applying new observations such as GRACE

622 follow-on and Surface Water and Ocean Topography (SWOT), sensitivity analysis regarding  
623 data uncertainties, and the impacts of GRACE data assimilation on non-assimilated variables.

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