

1 **Improving estimates of water resources in a semi-arid region by assimilating GRACE
2 data into the PCR-GLOBWB hydrological model**

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21 **Abstract**

22 An accurate estimation of water resources dynamics is crucial for proper management of both
23 agriculture and the local ecology, particularly in semi-arid regions. Imperfections in model
24 physics, uncertainties in model land parameters and meteorological data, as well as the human
25 impact on land changes often limit the accuracy of hydrological models in estimating water
26 storages. To mitigate this problem, this study investigated the assimilation of Terrestrial
27 Water Storage Variation (TWSV) estimates derived from the Gravity Recovery And Climate
28 Experiment (GRACE) data using an Ensemble Kalman Filter (EnKF) approach. The region
29 considered was the Hexi Corridor in Northern China. The hydrological model used for the
30 analysis was PCR-GLOBWB, driven by satellite-based forcing data from April 2002 to
31 December 2010. The impact of the GRACE Data Assimilation (DA) scheme was evaluated in
32 terms of the TWSV, as well as the variation of individual hydrological storage estimates. The
33 capability of GRACE DA to adjust the storage level was apparent not only for the entire
34 TWSV but also for the groundwater component. In this study, spatially-correlated errors in
35 GRACE data were taken into account, utilizing the full error variance-covariance matrices
36 provided as a part of the GRACE data product. The benefits of this approach were
37 demonstrated by comparing the EnKF results obtained with and without taking into account
38 error correlations. The results were validated against in situ groundwater data from 5 well
39 sites. On average, the experiments showed that GRACE DA improved the accuracy of
40 groundwater storage estimates by as much as 25%. The inclusion of error correlations
41 provided an equal or greater improvement in the estimates. In contrast, a validation against in
42 situ streamflow data from two river gauges showed no significant benefits of GRACE DA.

43 This is likely due to the limited spatial and temporal resolution of GRACE observations.
44 Finally, results of the GRACE DA study were used to assess the status of water resources
45 over the Hexi Corridor over the considered 9-year time interval. A really-averaged values
46 revealed that TWS, soil moisture, and groundwater storages over the region decreased with an
47 average rate of approximately 0.2, 0.1, and 0.1 cm/yr in terms of equivalent water heights,
48 respectively. A particularly rapid decline in TWS (approximately -0.4 cm/yr) was seen over
49 the Shiyang River Basin located in the southeaster part of Hexi Corridor. The reduction
50 mostly occurred in the groundwater layer. An investigation of the relationship between water
51 resources and agricultural activities suggested that groundwater consumption required to
52 maintain crop yield in the growing season for this specific basin was likely the cause of the
53 groundwater depletion.

54

55 **1. Introduction**

56 The focus of this study is the Hexi Corridor. It is a semi-arid region located between the
57 Gansu province of China and Mongolia (Fig. 1). A semi-arid region can be broadly classified
58 as an area on the boundary of a larger desert, receiving just enough annual precipitation (300
59 mm or less) to sustain a limited amount of agriculture (Gong et al., 2004; Zhu et al., 2015).
60 Inefficient use of the limited amount of surface water can often lead to overuse of
61 groundwater resources and salinization of the soil (Cui and Shao, 2005). This can result in
62 desertification, which not only reduces the amount of production but also may have long-term
63 effects on the local ecology. All of this holds true for the Hexi Corridor (Wang et al., 2003).

64 Improving the water resources management of semi-arid regions requires accurate knowledge
65 of the hydrological processes involved. For small areas, this can be partially obtained through
66 a network of in-situ measurement systems, such as meteorological stations, river gauges,
67 groundwater wells, evaporation trays, etc. (Dahlgren & Possling, 2007; Huo et al., 2007;
68 Kang et al., 2004; Ma et al., 2005; Du et al., 2014). While streamflow gauges provide
69 integrated information for large catchment areas, point observations of hydrometeorological
70 variables and even groundwater levels can be very local in scope. A sensor at a point several
71 kilometres away may record significantly different values. For large scales ($> 10,000$ km 2),
72 such techniques are unlikely capable of delivering accurate results.

73 Two options for estimating the large-scale Terrestrial Water Storage Variation (TWSV) of a
74 particular region are using observations from the Gravity Recovery And Climate Experiment
75 satellite mission (GRACE, Tapley et al., 2004) or utilizing a regional or global hydrological
76 model. A number of prior studies have reported on the potential of GRACE in the estimation
77 of snow water equivalent (Niu et al., 2007), groundwater (Döll et al., 2014), and
78 evapotranspiration (Long et al., 2014) in terms of temporal and spatial variability. However,
79 GRACE only provides the total column of the water storage at a monthly time scale and large
80 spatial scales (> 300 km). It is not possible to identify the contribution of separate
81 hydrological components to the TWSV from GRACE data alone. On the other hand, a
82 hydrological model can be used to estimate the individual storage components at very high
83 spatial and temporal scales. The major drawback of the model approach is mainly the

84 significant uncertainties influenced by the quality of the model parameter calibration and the
85 accuracy of the meteorological input data. In addition, hydrological models may suffer from
86 inadequate process representations (model structure errors).

87 Data Assimilation (DA) can be employed to combine the strengths of GRACE and
88 hydrological models while mitigating their respective weaknesses. A number of studies have
89 shown that GRACE DA can be used to improve the estimation of groundwater and
90 streamflow (Zaitchik et al., 2008; Tangdamrongsub et al., 2015), snow water equivalent
91 (Forman et al., 2012; Su et al., 2012), and as well as for evaluation of drought events
92 (Houborg et al., 2012; Li et al., 2012). Different temporal and spatial resolution of GRACE
93 observations and hydrological models require proper design of the DA scheme. Several DA
94 schemes have been developed to distribute GRACE observations into the model, which
95 include using 5-day interpolated observations and updating the model every 5 days
96 (Tangdamrongsub et al., 2015); using a monthly observation value and applying the model
97 update only at the end of the month (Eicker et al., 2014); using a monthly value and
98 distributing the update as a daily increments (Zaitchik et al., 2008; Forman et al., 2012;
99 Girotto et al. 2016). Although all DA schemes are acceptable, the scheme proposed by
100 Forman et al. (2012) is advantageous because it does not require an interpolation of the
101 observations and can reduce the spurious jump of the water storage estimates caused by
102 applying the update at the end of the month only. The only price to pay is the additional
103 computational cost of running the model twice for the same month. A scheme similar to
104 (Forman et al., 2012) is used in this study. Spatial disaggregation is also needed to reconcile
105 the difference in horizontal resolution between the observations and the model. Recent studies
106 by Eicker et al. (2014) and Schumacher et al. (2016) suggested including the GRACE
107 variance-covariance error information in the spatial disaggregation step. Both studies
108 proposed using 500-km GRACE spatial resolution to mitigate the ill-posedness of the error
109 covariance matrices in the spatial domain. In line with Eicker et al. (2014) and Schumacher et
110 al. (2016), the assimilation scheme in this study accounts for spatially correlated errors by
111 using full error variance-covariance matrices of GRACE data. This study will show that
112 considering the GRACE error correlations leads to an improvement of the state estimates.
113 Particularly, the Signal-to-Noise Ratio (SNR) of the TWSV is much lower than in the river
114 basins considered in the previous studies, e.g., Mississippi (Zaitchik et al., 2008), Rhine
115 (Tangdamrongsub et al., 2015), and Mackenzie (Forman et al., 2012).

116 Approximately 9 years of GRACE data – between April 2002 and December 2010 – are
117 considered in this study. GRACE observations are assimilated into the PCRaster Global
118 Water Balance (PCR-GLOBWB; Van Beek et al., 2011; Sutanudjaja et al., 2014; Wada et al.,
119 2014) hydrological model over the Hexi Corridor. TWS is computed from PCR-GLOBWB as
120 the sum of all the hydrological components (soil moisture, groundwater, surface water,
121 inundated water, interception, and snow). The previous studies showed very good agreement
122 of PCR-GLOBWB based estimates with GRACE observations in several river basins (Wada
123 et al., 2014; Tangdamrongsub et al., 2016). However, the performance of PCR-GLOBWB has
124 not yet been evaluated over the Hexi Corridor. In addition, to date the model has not been
125 incorporated into any GRACE DA scheme, making this study the first attempt to do so.

126 Investigating the added value of GRACE DA in the Hexi Corridor is the main objective of
127 this study.

128 First of all, the impact of GRACE DA and the effect of taking correlations in GRACE errors
129 into account are assessed. Both the total terrestrial water storage and the individual
130 hydrological storage compartments are considered.

131 Next, the results of the GRACE DA are validated with independent in-situ data. The
132 agreement is analysed in terms of the correlation coefficient, Nash-Sutcliff coefficient, and
133 Root-Mean-Square difference (RMSD). The groundwater storage variation (GWSV) and
134 streamflow estimates after GRACE DA are validated with the well and river stream gauge
135 measurements, respectively.

136 Finally, results from this GRACE DA study are used to assess the status of water resources
137 over the Hexi Corridor. The connections between the water storage (including groundwater
138 consumption) and agriculture in the area are also presented and discussed. At that stage, we
139 use precipitation data from the Tropical Rainfall Measuring Mission (TRMM; Huffman et al.,
140 2007) and the Moderate Resolution Imaging Spectroradiometer (MODIS) derived Normalized
141 Difference Vegetation Index (NDVI; Huete et al., 2002).

142

143 **2. Study region**

144 The Hexi Corridor is a long and narrow area between the Qilian Mountain range and southern
145 Mongolia (Fig. 1a). The region's elevation ranges from 5,200 m in the southern upstream area
146 (Qilian Mountains) to 900 m in the northern downstream zone (Inner Mongolia) (Fig. 1b).
147 The region is comprised of four typical inland arid and semi-arid regions (Zhu et al., 2015):
148 the Shiyang River Basin ($41,600 \text{ km}^2$), the Heihe River Basin ($143,000 \text{ km}^2$), the Shule River
149 Basin ($157,000 \text{ km}^2$), and a Desert Region ($152,445 \text{ km}^2$) (Geng and Wardlaw, 2013; Zhu et
150 al., 2015). Located next to the Gobi Desert, most parts of the region have a cold desert climate
151 (Peel et al., 2007), where precipitation is relatively low to sustain vegetation or crops.

152 Approximately 60 to 80 % of the annual rainfall is concentrated during the timeframe from
153 June to September. The inland rivers mainly originate from the Qilian Mountains and
154 disappear after entering the midstream/downstream plains and oases. As such, the southern
155 part of the region is more favourable for agriculture.

156 The four basins have distinct characteristics. First, the smallest river basin, Shiyang, has 8
157 main river streams, including the Xida and Xiying Rivers (Fig. 1c). The annual rainfall and
158 the mean temperature are approximately 250 mm and 5 °C (Fig. 2a, b), respectively. The
159 Shiyang River Basin is considered the wettest basin compared to the others, with relatively
160 high mean total renewable annual water resources of approximately 1.66 billion m^3 (Zheng et
161 al., 2013). However, a highly developed economy and population growth in the past decade
162 have resulted in a severe water resources overexploitation problem (Zheng et al., 2013). The
163 Heihe River Basin has a semi-arid climate and the mean daily temperature of ~6 °C (Fig. 2d).
164 The average annual rainfall is ~150 mm (Fig. 2c) with high heterogeneity both in temporal

165 and spatial distribution. The mean total annual available water resources are estimated at 3.7
166 billion m³ (Hu, 2015). Similar to the Shiyang River Basin, increased water exploitation,
167 increasing population, and changing climate have aggravated the damage to the downstream
168 ecology. The Shule River Basin has an arid climate, the mean temperature there is around 4
169 °C (Fig. 2f), and the average annual rainfall is only approximately 98 mm (Fig. 2e).
170 Compared to the Shiyang River Basin, the Shule River Basin is approximately four times as
171 large in terms of surface area, but has similar mean total annual water resources, ~1.6 billion
172 m³ (Hu, 2015). The district irrigation areas are mainly located in the middle of the Shule
173 River Basin. Agricultural water consumption accounts for more than 80% of the total water
174 use. Finally, the Desert Region has an extreme continental desert climate with an average
175 temperature of 8 °C, and the annual rainfall of ~130 mm. Extensive groundwater abstraction
176 was also observed over the region (Jiao et al., 2015).

177

178 **3. Hydrology model**

179 The global distributed hydrological model PCR-GLOBWB (van Beek et al., 2011;
180 Sutanudjaja et al., 2016) simulates spatial and temporal continuous fields of fluxes and
181 storages in various water storage components (soil moisture, groundwater, surface water,
182 inundated water, interception, and snow). The model version used here (Sutanudjaja et al.,
183 2016) has a spatial resolution of 30 arc minutes (approximately 50 km at the equator), and a
184 temporal resolution of 1 day. Figure 3 illustrates the structure of PCR-GLOBWB model. The
185 model includes 2 soil layers (SM_{upp}, SM_{low}), an underlying hydrologically active and
186 replenishable groundwater (GWS_{active}) layer, a non-renewable groundwater (GWS_{fossil}) layer,
187 as well as interception, surface water, and snow stores. The non-renewable groundwater is
188 available for abstraction to satisfy water demands once the overlying hydrologically active
189 groundwater storage is depleted. For soil, snow, inundated top water, and interception stores,
190 an individual grid cell is divided into sub-grids associated with different types of topography,
191 vegetation phenology, and soil properties, as well as land cover types. Specifically, there are 4
192 types of land covers defined: short natural vegetation, tall natural vegetation, irrigated non-
193 paddy field, and irrigated paddy field. Soil components include the upper layer (SM_{upp}, 0 – 30
194 cm) and the lower layer (SM_{low}, 30 – 150 cm). The snow component includes snow water
195 equivalent (SWE), as well as snow free water (SFW) representing the storage of melted snow.
196 The water stored in the stream channels and lakes is also included in the TWS estimate. Based
197 on the structure of PCR-GLOBWB, the total water storage (TWS) is computed as the sum of
198 27 different water storage components: 8 soil moisture layers, 2 groundwater layers, 4
199 interception layers, 8 snow layers, 4 inundated top water layers, and 1 surface water layer.

200 For each grid cell and for each daily time step, the model determines the water balance in two
201 vertically stacked soil layers and the groundwater store. The model also computes the vertical
202 water exchanges between the soil layers and between the inundated top water layer and the
203 atmosphere, i.e. rainfall and snowmelt, percolation and capillary rise, as well as evaporation
204 and transpiration fluxes. The active groundwater store underlies the soil, is fed by net
205 groundwater recharge, discharges to baseflow as a linear reservoir, and is exempt from the

206 direct influence of evaporation and transpiration fluxes. However, capillary rise from the
 207 active groundwater store can occur depending on the simulated groundwater storage, the soil
 208 moisture deficit, and the unsaturated hydraulic conductivity. Fluxes are simulated according
 209 to the different land cover types. The model includes a physically-based scheme for
 210 infiltration and runoff, resulting in the direct runoff, interflow, as well as groundwater
 211 baseflow and recharge. River discharge is calculated by accumulating and routing the specific
 212 runoff along the drainage network. For further details, including model parameterization, the
 213 reader is referred to the technical reports and other relevant publications (van Beek and
 214 Bierkens, 2009; van Beek, 2008; Sutanudjaja et al., 2011, 2014).

215

216 4. Data and data processing

217 4.1 GRACE data

218 The GRACE gravity product release 5 (RL05), generated by the University of Texas at
 219 Austin's Center for Space Research (CSR, Bettadpur, 2012), was used as input. The product
 220 consists of monthly sets of spherical harmonic coefficients (SHC) complete to degree and
 221 order 60. On this basis, TWSVs were obtained for the study period between April 2002 and
 222 December 2010. The GRACE data were further processed in this study as follows:

- 223 • SHCs of degree 1 provided by Swenson et al. (2008) were restored, and all 5
 224 coefficients of degree 2 were replaced by the values estimated from satellite laser
 225 ranging (Cheng and Tapley, 2004).
- 226 • SHC variations were computed by removing the long-term mean (computed between
 227 April 2002 and December 2010) from each monthly solution.
- 228 • A destriping filter (Swenson and Wahr, 2006) was applied to the SHC variations. The
 229 filter used a 5th degree polynomial (Savitsky-Golay) over a 5-point window to remove
 230 the correlations; orders below 8 remained unchanged.
- 231 • An additional 250-km radius Gaussian smoothing (Jekeli, 1981) was applied to SHC
 232 variations to suppress high-frequency noise, and the TWS variations ($\Delta\sigma$ [m]) were
 233 then computed using (Wahr et al 1998)

$$234 \Delta\sigma(\theta, \phi) = \sum_{l=1}^{60} \sum_{m=-l}^l W_l \frac{s_l}{\frac{a_e(2l+1)}{3(1+k_l)} \frac{\rho_e}{\rho_w}} \Delta\bar{C}_{lm} \hat{Y}_{lm}(\theta, \phi), \quad (1)$$

235

236 where θ, ϕ are co-latitude and longitude in spherical coordinates, $\Delta\bar{C}_{lm}$ is the SHC
 237 variations of degree l and order m , \hat{Y}_{lm} is the normalized surface spherical harmonic,
 238 W_l is the Gaussian smoothing function, S_l is a scaling factor used to convert
 239 dimensionless coefficients to TWS in terms of Equivalent Water Heights (EWH), a_e
 240 is the semi-major axis of the reference ellipsoid, k_l is the load love number of degree
 241 l , ρ_e and ρ_w are the average density of the Earth and water, respectively. In this study,
 242 the TWS variations were computed at every 0.5°x0.5° grid cell. This cell size was
 243 selected through trial and error as a balance between performance and resolution.

243 In general, filters suppress not only noise but also the genuine TWSV signal, and are a well-
244 known source of signal leakage. To address this, a signal restoration method (Chen et al.,
245 2014; Tangdamrongsub et al., 2016) was employed. The method iteratively determined the
246 possible signal reduction caused by the Gaussian filter applied and added it back to the
247 filtered signals. The errors of the procedure grew with the number of iterations, requiring a
248 proper selection of the convergence criterion. In this study, the criterion was chosen
249 empirically: the signal restoration process was iteratively repeated until the increment in every
250 grid cell inside the Hexi Corridor became smaller than 0.5 cm. This value is 2-3 times smaller
251 than the GRACE uncertainty (Wahr et al., 2006; Klees et al., 2008; Dahle et al., 2014). Figure
252 4 demonstrates the signal restoration for October 2002. The convergence criterion was met
253 after approximately 6 iterations. The signal over the mountain range and Inner Mongolia
254 became apparent after the signal restoration was applied (see Fig. 4f).

255 **4.2 Forcing data**

256 The forcing data required by PCR-GLOBWB are precipitation, air temperature, and potential
257 evapotranspiration. Tangdamrongsub et al. (2015) showed that the use of high-quality
258 precipitation data might lead to better estimates of hydrological fluxes (e.g., TWSV and
259 streamflow). In principle, local precipitation and surface temperature measurements could be
260 obtained from the China Daily Ground Climate Dataset provided by the China Meteorological
261 Data Sharing Service System (<http://cdc.cma.gov.cn/home.do>). A total of 23 weather stations
262 were found over the Hexi Corridor (see Fig. 1b). However, the measurements were spatially
263 sparse and did not cover the entire region. Therefore, the global precipitation data were used
264 to achieve a better spatial coverage. Four global precipitation products were considered for
265 inclusion:

- 266 • The European Centre for Medium-range Weather Forecasts (ERA-Interim, spatial
267 resolution: $0.75^\circ \times 0.75^\circ$; Dee et al., 2011)
- 268 • The Tropical Rainfall Measuring Mission (TRMM 3B42, spatial resolution: 0.25°
269 $\times 0.25^\circ$; Huffman et al., 2007; Kummerow et al., 1998)
- 270 • The Climate Research Unit dataset (CRU, spatial resolution: $0.5^\circ \times 0.5^\circ$; Mitchell and
271 Jones, 2005; van Beek, 2008)
- 272 • The Princeton's Global Meteorological Forcing Dataset (Princeton, spatial resolution:
273 $0.5^\circ \times 0.5^\circ$; Sheffield et al., 2005)

274 To select the best product, the global precipitation values were first interpolated to the
275 weather station locations and then the correlation coefficient, Nash-Sutcliffe (NS) coefficient,
276 and RMSD between the interpolated and observed ground data were calculated. The mean
277 values of the statistical estimates are shown in Fig. 5a. Overall, TRMM provided the best data
278 quality, with the highest correlation (~0.85) and NS coefficients (~0.46), and an RMSD
279 approximately 2–3 mm lower than other products. The high spatial resolution of TRMM is
280 probably the reason for its better performance. Therefore, this product was chosen as the
281 precipitation input. The low NS coefficient in all 4 cases suggests that the coarse spatial
282 resolution of the global precipitation datasets prevents them from capturing all the local
283 precipitation events.

284 A similar procedure was used to compare the air temperature data from ERA-Interim, CRU,
285 and Princeton. The statistical estimates are shown in Fig. 5b. Although the results from all
286 products were very similar, CRU provided the highest data quality in terms of correlation and
287 RMSD values, and therefore, it was used as the temperature input. As far as potential
288 evapotranspiration is concerned, few data are available for this region, so the data from (van
289 Beek, 2008) were used.

290 **4.3 Validation data**

291 **4.3.1 Groundwater**

292 Monthly groundwater well measurements at 5 locations (Fig. 1c) were obtained from the
293 ground network maintained by the Shiyang River Basin Management Bureau, and Institute of
294 Water Resources and Hydropower of Gansu Province. The in situ data were provided in the
295 form of piezometric heads (relative to the mean sea level), which needed to be converted to
296 units of storage. For such a task, several parameters, e.g., storage coefficient and specific
297 yield are required, but they are not available over the Hexi Corridor. To solve that problem, a
298 scale factor computed using the information from GRACE and soil moisture (SM) from the
299 Global Land Data Assimilation System (GLDAS, Rodell et al., 2004) was used for the
300 conversion using the approach outlined by Tangdamrongsub et al. (2015). As discussed in
301 Tangdamrongsub et al. (2015), it is ideally preferred to use the in-situ soil moisture data to
302 represent the SM term, but they are not available at the well locations. The soil moisture
303 estimated from remote sensing was also not appropriate due to the limitation of the
304 penetration depth. The use of SM from PCR-GLOBWB is avoided to reduce the bias when
305 compared the adjusted well measurements to the final DA result. Therefore, the GLDAS
306 derived SM was used.

307 The adjustment procedure was as follows. First, GLDAS-based soil moisture storage
308 variations (SMSV) were removed from GRACE-derived TWSV. Four variants of GLDAS
309 model (NOAH, CLM, MOSAIC, and VIC; see Rodell et al., 2004) were considered and the
310 average SMSV value was calculated. Taking into account that SMSV and groundwater
311 storage variations (GWSV) are the major contributions to TWS variations, this resulted in
312 GWSV (GWSV_(GRACE-SMSV)). Then, by conducting a regression analysis between the monthly
313 time-series of piezometric head variation (Δh) and $\Delta GWS_{(GRACE-SMSV)}$ at each individual
314 location, a bias (b) and a scale factor (f) were estimated using the following linear
315 relationship:

316
$$\Delta GWS_{(GRACE-SMSV)} + e = b + f \cdot \Delta h, \quad (2)$$

317 where e indicates the observation error. Finally, the estimated bias (\hat{b}) and scale factor (\hat{f})
318 were used to convert the in situ head measurements into groundwater storage variation
319 (GWSV_{in situ}) as:

320
$$GWSV_{in situ} = \hat{b} + \hat{f} \cdot \Delta h. \quad (3)$$

321

322 **4.3.2 Streamflow**

323 Monthly river gauge data were obtained from the same data centre as the groundwater
324 measurements. Due to the coarse spatial resolution of PCR-GLOBWB, it models only the
325 main river streams. Therefore, the gauge measurements of small river streams, as well as the
326 gauge measurements that contained many data gaps (i.e., more than 24 months), were
327 excluded. As a result, the measurements from only 2 gauges – at Xida and Xiying Rivers (see
328 Fig. 1c) – were used in this study.

329 **4.4.3 Normalized Difference Vegetation Index (NDVI)**

330 NDVI (Carlson and Ripley, 1997) is an indicator of vegetation health or “greenness”. In this
331 study, NDVI and GWS were analysed to determine if the growing season was being extended
332 beyond the limited rainy period through groundwater extraction for irrigation. NDVI was
333 computed from the MODIS 8-day, 500-m spatial resolution surface reflectance product
334 (Vermote et al., 2011) based on data from Aqua satellite (MYD09A1 product). Based on the
335 location of the in situ groundwater measurements, the MODIS tiles h25v05 and h26v05 were
336 selected. First, the data were quality controlled to exclude pixels with cloud cover. The 8-day
337 NDVI was then computed as (Huete et al., 2002)

338
$$NDVI = \frac{\rho_{NIR} - \rho_R}{\rho_{NIR} + \rho_R}, \quad (4)$$

339 where ρ_{NIR} and ρ_R are the observed surface reflectances in the near-infrared and red portions
340 of the electromagnetic spectrum, respectively. The monthly-averaged NDVI was then
341 computed based on the derived 8-day NDVI values.

342

343 **5. Methodology and implementation**

344 **5.1 Ensemble Kalman Filter (EnKF)**

345 The Ensemble Kalman Filter (EnKF; Evensen, 2003) is used to assimilate GRACE derived
346 TWSV into the PCR-GLOBWB model. The EnKF works in two steps, a forecast step and
347 analysis (update) step. The forecast step involves propagating the states forward in time using
348 the model (PCR-GLOBWB). Identical to how the EnKF is implemented by Forman et al.
349 (2012), the state vector (ψ in this study) is an $nm \times 1$ vector, where $n = 27$ is the number of
350 TWS-related states from PCR-GLOBWB (see Sect. 3), and m is the number of model grid
351 cells. The model estimates are related to the GRACE observations by

352
$$\mathbf{d} = \mathbf{H}\psi + \boldsymbol{\epsilon}; \boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{R}), \quad (5)$$

353 where \mathbf{d} is an $m \times 1$ vector containing the GRACE observations for the month of interest, and
354 \mathbf{H} is a measurement operator which relates the PCR-GLOBWB state ψ to the observation
355 vector \mathbf{d} . Notice that the number of observations is equal to the number of grid cells because
356 the GRACE-based estimates are obtained for all the grid cells of the PCR-GLOBWB model
357 (see Sect. 4.1). The uncertainties in the observations are given in the random error $\boldsymbol{\epsilon}$, which is

358 assumed to have zero mean and covariance matrix $\mathbf{R}_{m \times m}$. As the sum of all state elements at
 359 a given cell is equal to TWSV, the \mathbf{H} matrix is defined as:

$$360 \quad \mathbf{H} = \left[\begin{pmatrix} (1 1 1 \dots 1)_{1 \times n} & 0 & \dots & 0 \\ 0 & (1 1 1 \dots 1)_{1 \times n} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & (1 1 1 \dots 1)_{1 \times n} \end{pmatrix} \right]_{m \times nm}. \quad (6)$$

361 Let the ensemble of the states be stored in a matrix $\mathbf{A}_{nm \times N} = (\boldsymbol{\psi}_1, \boldsymbol{\psi}_2, \boldsymbol{\psi}_3, \dots, \boldsymbol{\psi}_N)$, where N
 362 is the number of ensemble members. Then, the ensemble perturbation matrix is defined as
 363 $\mathbf{A}' = \mathbf{A} - \bar{\mathbf{A}}$, where the matrix $\bar{\mathbf{A}}$ is of the same size as \mathbf{A} and filled in with the mean values
 364 computed from all ensemble members. Similarly, the GRACE observation vector is stored in
 365 the matrix $\mathbf{D}_{m \times N} = (\mathbf{d}_1, \mathbf{d}_2, \mathbf{d}_3, \dots, \mathbf{d}_N)$, in which each column is a replicate of the
 366 observation but perturbed with random noise $\sim \mathcal{N}(\mathbf{0}, \mathbf{R})$. The analysis equation can be
 367 expressed as (Evensen, 2003)

$$368 \quad \mathbf{A}^a = \mathbf{A} + \Delta\mathbf{A} = \mathbf{A} + \mathbf{K}(\mathbf{D} - \mathbf{H}\mathbf{A}) \quad (7)$$

369 with

$$370 \quad \mathbf{K} = \mathbf{P}_e \mathbf{H}^T (\mathbf{H} \mathbf{P}_e \mathbf{H}^T + \mathbf{R})^{-1}, \quad (8)$$

371 where $\mathbf{A}_{nm \times N}^a$ is the updated model state, $\Delta\mathbf{A}_{nm \times N}$ is the update from Kalman filter, and
 372 $\mathbf{K}_{nm \times m}$ is the Kalman gain matrix. The model error covariance matrix $(\mathbf{P}_e)_{nm \times nm}$ is
 373 computed as

$$374 \quad \mathbf{P}_e = \mathbf{A}'(\mathbf{A}')^T / (N - 1). \quad (9)$$

375 The matrix \mathbf{R} is the error variance-covariance matrix of GRACE data in the spatial domain, its
 376 computation is discussed in Sect. 5.2.2.

377 In the initialization phase, which was needed to obtain the initial states, the model was spun
 378 up between 1 January 2000 and 31 December 2000 as a hot start. This time interval was
 379 sufficient to reach the dynamic equilibrium. The initial state $\boldsymbol{\psi}$ for 31 December 2000
 380 obtained this way was perturbed to yield $N = 100$ ensemble members $\boldsymbol{\psi}_i, i = 1, 2, 3, \dots, N$.
 381 The N ensemble runs between 1 January 2001 and 31 March 2002 were then conducted
 382 independently based on the perturbed initial states. This resulted in an ensemble spread of the
 383 estimated states. The model was then propagated in time between 1 April 2002 and 31
 384 December 2010 without assimilating any observation. This case is referred to hereafter as the
 385 Ensemble Open Loop (EnOL). For the EnKF, the model was also propagated beginning from
 386 1 April 2002, but the observations (when available) were assimilated.

387 The processing diagram is shown in Fig. 6, and follows the methodology introduced by
 388 Forman et al. (2012). The state is first propagated in time from the first to the last day of the
 389 month without applying DA, and the monthly averaged states are calculated from the daily
 390 values. When the GRACE observation for that month is available, the DA routine is activated
 391 (otherwise, the model continues propagating to the next month without applying DA). The

392 DA routine computes the monthly averaged update $\Delta\mathbf{A}$ of the TWS-related states, cf. Eq. (7).
 393 The daily increment (DINC) of the update is then computed by dividing the monthly averaged
 394 update by the total numbers of days in that month (numday_{month}). The model propagation is
 395 then restarted (second run), using the last day of the previous month (month-1, numday_{month-1})
 396 as the initial state. In this second run, the DINC is added to the current states every day up to
 397 the last day of the month. The DA scheme is repeated for each month up to the end of the
 398 study period.

399 Spatial correlations of model errors and observation errors were also taken into account in
 400 view of the fact that the latter are highly correlated at neighbouring $0.5^\circ \times 0.5^\circ$ grid cells. De
 401 Lannoy et al. (2009) proposed a so-called 3D-Fm (3-dimentional fine scale with multiple
 402 observation) approach, which is called EnKF 3D in this paper. The approach only considers
 403 the spatial correlations between the neighbouring grid cells. In this study, the neighbouring
 404 grid cells were assumed to be the ones inside the Gaussian smoothing radius applied, i.e., 250
 405 km. This reduced the computational cost, as only a small subset of cells pairs was considered
 406 instead of all cells pairs. That approach was applied not only to observation errors, but also to
 407 model errors in TWSV and TWS-related components in this study. The EnKF 3D scheme is
 408 illustrated in Fig. 7. For a particular grid cell (centre grid cell), all TWS-related components
 409 of the neighbouring grid cells and the centre grid cell are used to form the state ($\mathbf{A}^s_{np \times N}$) and
 410 observation ($\mathbf{D}^s_{p \times N}$) matrices, where p is the number of the considered grid cells. The matrix
 411 notation with superscript s (e.g., \mathbf{A}^s) is only used to emphasize the cell-dependent version, and
 412 it can be substituted into the original matrix notation (e.g., \mathbf{A}) in Eqs. (5–9). It is emphasized
 413 here that EnKF 3D involves only p grid cells instead of all m grid cells. As such, the
 414 measurement operator, model error covariance matrix, and observation error covariance
 415 matrix become $\mathbf{H}^s_{p \times np}$, $(\mathbf{P}_e^s)_{np \times np}$, and $\mathbf{R}^s_{p \times p}$, respectively. The EnKF was then applied and
 416 the states of the centre grid cell (only) were updated. The procedure was repeated through all
 417 grid cells. To investigate the impact of including spatial correlations of errors, the EnKF 1D
 418 was also considered. The EnKF 1D scheme is similar to EnKF 3D, but the spatial correlations
 419 are omitted (i.e., the off-diagonal elements of the covariance matrices \mathbf{P}_e^s and \mathbf{R}^s are set to
 420 zero).

421 Furthermore, sampling errors caused by finite ensemble size might lead to spurious
 422 correlations in the estimated model error covariance matrices (Hamill et al., 2001). To reduce
 423 such an effect, a distance-dependent localization function is applied to \mathbf{P}_e^s (pair-wise). In this
 424 study, the Gaussian function ($c(\alpha)$) (Jekeli, 1981) was used for that:

$$425 \quad c(\alpha_{j_1, j_2}) = \frac{e^{-b[1-\cos(\alpha_{j_1, j_2}/a_e)]}}{1-e^{-2b}} \quad (10)$$

$$426 \quad \text{with } b = \frac{\ln(2)}{1-\cos(L/a_e)}, \quad (11)$$

427 where α_{j_1, j_2} is the distance on the Earth's surface between two grid cells (j_1 and j_2), and L is
 428 the correlation distance. The variogram analysis was used to derive the TWSV correlation
 429 distance (L) of PCR-GLOBWB, assuming that it is similar to the correlation distance of
 430 model errors. It was found to be approximately equal to 110 km over the Hexi Corridor. For

431 GRACE observations, to ensure that the spurious error correlations at distances greater than
432 the Gaussian smoothing distance, 250 km, are insignificant, the localization applied to \mathbf{R}^s was
433 based on $L = 250$ km. The localization also makes the correlations at short distances slightly
434 weaker. As a result, the condition number of the error covariance matrix is increased. In this
435 study, for instance, the condition number increased from $\sim 10^{14}$ to $\sim 10^2$. Thus, this matrix had
436 a full rank after localization (see Sect. 5.2.2 for a further discussion).

437

438 **5.2 Errors of PCR-GLOBWB model and errors in GRACE observations**

439 **5.2.1 Model errors**

440 The two primary sources of considered errors in the PCR-GLOBWB model are the
441 meteorological forcing data and the model parameters. For forcing data, the precipitation
442 uncertainties were quantified as the RMS error provided by the TRMM product (Huffman,
443 1997). The uncertainties of temperature and potential evapotranspiration were not provided as
444 parts of the corresponding products, and therefore errors of 2°C, and 30% of the nominal
445 potential evapotranspiration value were assumed, respectively. The error levels were chosen
446 through trial-and-error, mainly to allow the ensemble to grow between updates. The
447 precipitation and potential evapotranspiration were perturbed with additive lognormal noise
448 while the temperature was perturbed with additive Gaussian noise. The forcing data
449 uncertainties were assumed to be spatially correlated, which was accounted for using an
450 exponential decay function. Based on a variogram analysis, the correlation distances of
451 precipitation, temperature and potential evapotranspiration were found to be approximately
452 150 km, 450 km, and 450 km, respectively.

453 As far as model parameters are concerned, a total of 15 TWS-related parameters (see Table 1,
454 Sutanudjaja et al., 2011, 2014) were perturbed using additive Gaussian noise without spatial
455 correlations. The standard deviation of the perturbations of the parameters was set to 20% of
456 the range of the nominal values.

457 **5.2.2 GRACE observation errors**

458 Spatial correlations of GRACE observation errors were also taken into account in the DA
459 scheme. The uncertainties in the GRACE-derived TWSV over the Hexi Corridor were
460 computed using the monthly calibrated error variance-covariance matrix of the SHCs (Σ)
461 provided by the CSR. Recalling the replacement of the low degree SHCs (see Sect. 4.1), the
462 error (co-)variances of SHCs degree 2 were not provided by Cheng and Tapley (2004), and
463 therefore the values obtained from the CSR were used. As for SHCs of degree 1, the error (co-
464) variances were not available from (Swenson et al., 2008) either and were set to zero. Note
465 that Σ only reflects the error of the original GRACE data, i.e. before the GRACE processing
466 described in Sect. 4.1 was applied. To obtain the error variance-covariance matrix associated
467 with the post-processed GRACE data, an ensemble of SHC noise realizations \mathbf{Q}^c was first
468 generated based on Σ as follows:

469 $\mathbf{Q}^c = (\Sigma)^{\frac{1}{2}} \mathbf{Q}^w,$ (12)

470 where $\mathbf{Q}^w = (q_1^w, q_2^w, q_3^w, \dots, q_N^w)$ contains a set of white noise realizations and has the
 471 dimension of $s \times N$, where $s = 1891$ is the number of SHCs, and $N = 100$ is the number of
 472 realizations. The matrix $\mathbf{Q}^c = (q_1^c, q_2^c, q_3^c, \dots, q_N^c)$ has the same dimension as \mathbf{Q}^w and contains
 473 an ensemble of correlated noise realizations in SHCs. Then, each noise realization (i.e.,
 474 column of \mathbf{Q}^c) was post-processed in the same way as the GRACE data (Sect. 4.1), which
 475 resulted in $\widehat{\mathbf{Q}}^c = (\widehat{q}_1^c, \widehat{q}_2^c, \widehat{q}_3^c, \dots, \widehat{q}_N^c)$. The post-processing included applying the destriping and
 476 Gaussian smoothing filters, as well as the signal restoration using the same number of
 477 iterations as was used in the GRACE data post-processing. The error variance-covariance
 478 matrix $\widehat{\Sigma}$ associated with the SHCs after post-processing was then computed as

479 $\widehat{\Sigma} = [\widehat{\mathbf{Q}}^c (\widehat{\mathbf{Q}}^c)^T] / (N - 1).$ (13)

480 Recalling Eq. (1), the TWSV over the Hexi Corridor can be computed as

481 $\Delta\sigma = \mathbf{Y}\mathbf{S}\mathbf{x},$ (14)

482 where $\Delta\sigma$ is the vector composed of the computed TWSV at grid cells, \mathbf{Y} is the matrix of
 483 spherical harmonic synthesis (cf. Eq. (1)), \mathbf{S} is the matrix containing the scaling factors S_l , and
 484 \mathbf{x} is the vector composed of the dimensionless SHC variations after GRACE data post-
 485 processing described in Sect. 4.1. Then, the error covariance matrix \mathbf{R} of the GRACE-based
 486 TWSV over the Hexi Corridor was computed with the error propagation law as

487 $\mathbf{R} = \mathbf{Y}\mathbf{S}\widehat{\Sigma}(\mathbf{Y}\mathbf{S})^T.$ (15)

488 Some statistics of GRACE TWSV errors over the Hexi Corridor are shown in Fig. 8. The
 489 error standard deviation in Oct. 2002 varied with location (Fig. 8a), whereas the error
 490 correlation showed a distance-decay pattern in all directions (Fig. 8b). The areally-averaged
 491 standard deviations over 4 basins stayed in most of the months at a similar level of
 492 approximately 1 cm (Fig. 8c). The large uncertainty in September 2004 was likely caused by
 493 the near-repeat orbit of GRACE satellites during that month.

494

495 **6. Results and discussion**

496 The structure of this section is as follows. First, the impact of assimilation using EnKF 3D on
 497 the TWSV is considered in Sect. 6.1. Then, the impact of the EnKF 3D on the estimates of the
 498 individual stores is investigated in Sect. 6.2. The results of the EnKF 1D and EnKF 3D
 499 schemes are compared in Sect. 6.3 in terms of TWSV and the individual stores. Furthermore,
 500 the obtained results are validated against independent data in Sect. 6.4. Finally, in Sect. 6.5-
 501 6.6, the assimilation results are used together with ancillary remote sensing data to study
 502 water resources in the Hexi Corridor.

503

504 **6.1 Impact of GRACE DA**

505 To demonstrate the impact of DA, Fig. 9 shows the daily TWSV estimates over the Shiyang
506 River Basin between 1 April 2002 and 31 December 2003. Several features associated with
507 the EnKF can be observed. Firstly, when a GRACE observation is available, the EnKF moves
508 the estimated TWSV towards it. As a result, the estimated TWSV lies between the EnOL
509 estimate and the GRACE observation most of the time. It is seen that GRACE-derived TWSV
510 has a greater annual amplitude compared to the model estimated TWSV. This can likely be
511 attributed to the poor quality of the model parameter calibration and the accuracy of the
512 meteorological input data over the data-sparse regions. In the absence of observations, model
513 parameters are difficult to determine and only the best available knowledge (or guess) is
514 generally used, leading to inaccurate model state estimates. Updating the water storage
515 estimates using GRACE DA showed a clear improvement in this case. Secondly, the standard
516 deviation across the EnKF ensemble of TWSV values is smaller than that of the EnOL and
517 smaller than the GRACE observation error. Thirdly, at the first month (April 2002) the
518 TWSV estimates of the EnOL and EnKF were similar at the forecast step (as the initial states
519 were the same, see point (a) in Fig. 9), but became different when the daily increment was
520 applied to the EnKF. Finally, discontinuities in the time-series before the update were
521 observed at the end of the month e.g., in November and December 2002 (point (b) and (c)),
522 and February 2003 (point (d)). Applying the daily increment (see Sect. 5.3) served as a
523 smoother, and these stepwise changes were reduced.

524 Similar features were also seen in the EnKF 1D TWSV estimates (not shown).

525

526 **6.2 Impact of GRACE DA on individual stores**

527 The monthly-averaged values of the TWSV and individual stores in each of the 4 basins are
528 presented in Fig. 10. Overall, TWSV estimates over the Hexi Corridor mostly reflect SMSV
529 and GWSV components, while snow water storage variation (SNSV) and surface water
530 storage variation (SFWV) are minor contributors, constituting less than 5% in most basins.
531 Clear seasonal variations in TWSV were seen in all basins for GRACE, EnOL and GRACE
532 DA (both EnKF 1D and EnKF 3D) time-series (Fig. 10 a,b,c,d). As observed in Fig. 10, the
533 GRACE DA estimated TWSVs are generally between the GRACE observations and the
534 EnOL estimates. As a result of assimilating GRACE data, both the EnKF 1D and EnKF 3D
535 added water to all basins between 2002 and 2005 and reduced it from the basins between
536 2006 and 2010. This is also seen in the time-series of SMSV (Fig. 12 e,f,g,h) and GWSV
537 (Fig. 12 I,j,k,l). Additionally, the annual amplitudes and phases of GRACE DA estimated
538 TWSV were also found mostly in between the values computed from the GRACE
539 observations and the EnOL results (see Table 2). In particular, the GRACE-DA estimated
540 TWSV's phase was always closer to the GRACE observation. The phase shifts of
541 approximately 1 month were seen in both GRACE DA estimated TWS and GRACE
542 observations compared to the EnOL results. Similar phase differences of approximately 1
543 month were also observed in SMSV and GWSV components.

544 Differences in the long-term trends were also detected between the TWSV estimates from the
545 model alone (EnOL) and the GRACE DA. The GRACE DA results showed decreasing
546 TWSV trends similarly to the GRACE data, while the EnOL showed increasing trends (Fig.
547 10 a,b,c,d, see also Table 7). This change in TWSV trend was clearly a result of assimilating
548 GRACE observations. The negative trends were also observed after DA in the GWSV
549 component in most basins (Fig. 10 i,j,l). This indicates the potential of GRACE DA in
550 adjusting GWSV. In this way, one can reveal continued groundwater consumption to support
551 local agricultural activities (Li et al., 2013). Unlike over other basins, the negative trend of
552 GWSV estimates was not clearly present over the Desert Region (Fig.10k). This could be due
553 to the small amplitude of the groundwater variation of this region (see also below), and most
554 of the update took place in the SM component. As a result, a relatively large negative trend
555 was seen in SMSV rather than GWSV after GRACE DA (see also Table 7). Further
556 discussions on the trends are given in Sect. 6.4.

557 The impact of GRACE DA on different stores was influenced by both the model parameters
558 and the forcing data. The 4 basins have similar soil water storage capacities (see Table 3),
559 which indicates that the basins can store similar amounts of soil water and generate similar
560 amounts of groundwater recharge under the same rainfall conditions. However, the 4 basins
561 received different amounts of rainfall, which resulted in different SMSV and GWSV
562 estimates. For example, the Shiyang River Basin received the greatest amount of rainfall (~
563 twice of Heihe River Basin), which led to the greatest amount of the SMSV estimate (~1 cm
564 annual amplitude). Such a large amount was also sufficient to percolate into the groundwater
565 layer, resulting in GWSV of ~0.7 cm (see Fig. 10i and Table 2). In contrast, the Desert
566 Region received approximately 3 times less rainfall, which led to a somewhat smaller amount
567 of SMSV (~0.7 cm annual amplitude) and a much smaller amount of GWSV, ~0.2 cm (see
568 Fig. 10g, k). As the uncertainty of the water storage variation is associated with the signal
569 amplitude, the greater (smaller) water storage variation leads to greater (smaller) uncertainty,
570 resulting in greater (smaller) update from GRACE DA. As such, a greater update (in
571 particular, in GWSV) is seen over the Shiyang River Basin, as compared to other basins.

572 Snow estimates (SWE plus SFW) were very small (less than 0.2 cm) over the Hexi Corridor
573 and therefore were only slightly updated by GRACE DA. Note that the large variability in the
574 amount of snow seen as the sharp peaks (e.g., in January 2008) was caused by the
575 precipitation and temperature variability. In January 2008, the precipitation records were 159
576 % higher than the January average value while the temperature was 2 – 3°C lower. Such a
577 condition resulted in a large amount of snow. Finally, GRACE DA influences the surface
578 water, but the amplitude is still lower than that of the GRACE uncertainties. Validation of the
579 surface water estimates in terms of river streamflow is given in Sect. 6.4.2.

580

581 **6.3 Impact of taking spatial correlations of errors into account**

582 The impact of accounting for the error correlations was clearly seen in the TWSV estimates
583 (Fig. 10 a,b,c,d). When the error correlations were ignored (EnKF 1D), the TWSV estimate
584 received a larger update from GRACE, particularly between 2002 and 2005. Hence, the

585 estimate was drawn significantly closer to the observation. The presence of error correlations
586 effectively reduces the amount of information in the GRACE data, since spatial averaging of
587 such data mitigates noise to a much less extent than averaging of data with uncorrelated
588 errors. Therefore, the impact of GRACE data in the EnKF 3D case is reduced. As such, the
589 EnKF 3D estimated TWSV was always between the EnOL and EnKF 1D results. Validating
590 against the in situ groundwater and streamflow data will quantitatively reveal the performance
591 of each approach (Sect. 6.4).

592 Taking error correlations into account also has a clear impact on the SMSV and GWSV
593 components. For SMSV, similarly to TWSV, the EnKF 1D yielded a larger update between
594 2002 and 2005 compared to the EnKF 3D (Fig. 10 e,f,g,h). The difference between EnKF 1D
595 and 3D results became smaller after 2005. This can be attributed to the fact that the ensemble
596 spread in the soil moisture component becomes smaller after several years of updates. After
597 2005, the ensemble spread of SMS was lower than the GRACE uncertainty, and therefore
598 taking the error correlations into account did not have a significant impact on the SMS
599 estimates. For GWS, the impact of taking error correlations into account was even clearer,
600 especially in terms of the long-term trend (Fig. 10, i,j,k,l). With the exception of the Desert
601 Region, the EnKF 1D showed a steeper decreasing trend in all basins. For snow and surface
602 water, the impact of considering error correlations was not significant due to the fact that the
603 stores are small, as compared to SMS and GWS.

604 It is also worth discussing the impact of GRACE DA on the spatial pattern of the water
605 storage estimates. To demonstrate this, the update term (ΔA in Eq. (7)) of October 2002 from
606 EnKF 1D and 3D cases is shown in Fig. 11. Only TWSV, SMSV, and GWSV are presented,
607 since other components (snow, surface water, and interception) are small. As discussed above,
608 EnKF 3D shows smaller update in all components. Due to a greater amplitude of GRACE-
609 derived TWSV over northern and southern parts of the region (see Fig. 4), the update is
610 mostly seen there. Almost all update is limited to the soil moisture layer. Higher precipitation
611 is generally observed over the southern part, which leads to higher groundwater recharge (and
612 GWSV) over that region. As such, a GWSV update is clearly seen over the southern part of
613 the region.

614

615 **6.4 Validation against independent data**

616 **6.4.1 Validation of groundwater estimates against well data**

617 The GWSs estimated from GRACE DA were validated against the well measurements at 5
618 locations shown in Fig. 1c. Yang et al. (2001) showed that the specific yield values obtained
619 from the field measurements over the Shiyang River Basin was between 0.01 and 0.3.
620 Although the measurements were not collected at the well stations used in this study, the
621 values obtained can be used as a guidance of the specific yield of the Shiyang River Basin. In
622 this study, the head measurements were converted to storage unit with the approach described
623 in Sect. 4.3.1. The bias term in Eq. (3) was found to be very close to zero, as the variation
624 (mean removed) was used in the regression analysis. The estimated scale factor was 0.23,

625 0.04, 0.24, 0.25, and 0.32 at W1 – W5, respectively, which is in line with the values obtained
626 from the field measurement.

627 The GWSV estimate at each well location is shown in Fig. 12. Compared to the EnOL results,
628 GRACE DA results were visually closer to the well measurements at all 5 locations. The
629 EnKF 1D and EnKF 3D showed a noticeable difference at each location. The updated GWSV
630 estimates were evaluated in terms of the correlation coefficient, RMSD, and long-term trend
631 (Table 4, 5). Overall, the EnOL resulted in relatively poor correlation coefficients at most
632 stations (except station W1), with the average value of only 0.06. Clear improvements were
633 seen after GRACE DA was applied. The average correlation coefficient increased to
634 approximately 0.6 – 0.7. Although the EnKF 1D introduced a greater update than the EnKF
635 3D, it only showed higher correlation coefficients at stations W1 and W3. Applying the EnKF
636 3D led to correlation coefficients greater than 0.45 in all stations, and on average it improved
637 the correlation coefficient by approximately 0.1 over EnKF 1D. In terms of RMSD, applying
638 GRACE DA reduced the difference by approximately 15 – 25% compared to the EnOL.
639 Compared to EnKF 1D, the EnKF 3D significantly improved the RMSD in most stations. The
640 EnKF 1D only performed better than EnKF 3D at station W1, where it reduced the RMSD by
641 approximately 16 % compared to 8% reduction by the EnKF 3D. The noticeably low GWSV
642 observed by the well data at station W2 in the summers of 2007 and 2008 (Fig. 12b) was
643 probably caused by significant groundwater abstraction. These local features could not be
644 reproduced by the model and GRACE observations due to a limited spatial resolution. As a
645 result, neither of the EnKF algorithms could improve the GWSV estimates at the W2 location
646 during those periods.

647 The long-term trend estimated between 2007 and 2010 was also used to evaluate the impact of
648 GRACE DA and the effect of taking the error correlations into account (Table 5). The EnOL
649 trend estimates were considered poor as they showed the largest RMSD respected to the in
650 situ data. In fact, they were the least consistent with the in situ estimates at each individual
651 station. Similar to the results in terms of correlation coefficient and RMSD (see Table 4), the
652 EnKF 3D led to the largest improvement in the trend estimates (RMSD=0.54 compared to
653 0.93 after EnKF 1D). However, while the EnKF 3D showed closer long-term trends to the in
654 situ measurements at stations W2, W4, W5, the EnKF 1D produced better estimates at station
655 W1 and W3.

656 Thus, both EnKF 1D and 3D led to the improvement of the GWSV estimates in terms of all
657 metrics. In terms of the average results and at the majority of well locations, the EnKF 3D
658 provided more improvement than the EnKF 1D.

659

660 **6.4.2 Validation of streamflow estimates against river gauge data**

661 The streamflow estimates were validated against the river gauge measurements at locations
662 G1 and G2 (Fig 1c). Results are shown in Figure 13 and Table 6. Only modest improvements
663 in the streamflow estimates were observed in terms of the correlation coefficient, NS
664 coefficient, and RMSD. This behaviour is similar to what was observed previously for the

665 Rhine River Basin, when a different hydrology model and input data were used
666 (Tangdamrongsub et al., 2015). Figure 13 shows that taking error correlations into account
667 had little impact, i.e. similar streamflow estimates were seen for EnKF 1D and 3D results. At
668 location G1 (Fig. 13a), GRACE DA added more water to the stream channel between 2002
669 and 2006 and reduced it between 2008 and 2010. This behaviour is consistent with the TWSV
670 estimates discussed in Sect. 6.2. GRACE DA increased the correlation coefficient from 0.82
671 to 0.84, increased the NS coefficient from 0.65 to 0.69, and reduced the RMSD by
672 approximately 5 % (Table 6). A lesser improvement was observed at G2.

673 Comparing to the gauge measurements, both the EnOL and GRACE DA overestimated the
674 streamflow in September 2007 and September 2008 at G2. The sudden surge in the estimated
675 streamflow resulted from heavy rainfall recorded by precipitation data while the soil was,
676 according to the model, already saturated (Fig. 14). For example, in September 2007, the
677 second highest amount of SM storage in the record (~19.5 cm) was obtained when the third
678 largest amount of rainfall (~90 mm/month) was observed. Similarly, in September 2008, large
679 SM storage (~20 cm) and the heaviest rainfall (~100 mm/day) forced PCR-GLOBWB to
680 generate a large amount of streamflow. In both cases, the modelled streamflow significantly
681 exceeded the actual one observed at G2. Inaccurate precipitation data and model calibration
682 likely led to these discrepancies. GRACE DA was unable to reduce these spurious peaks due
683 to the limited spatial (~250 km) and temporal (1 month) resolution of GRACE data.

684

685 **6.5 Declining water storages in the Hexi Corridor**

686 The water resources situation over the Hexi Corridor was assessed using long-term trends
687 estimated from the 9-year EnKF 3D results. This DA variant is primarily discussed here as it
688 provided better agreement with well observations than the EnKF 1D (see Sect. 6.4.1). For
689 completeness, however, the values estimated from GRACE, EnOL, EnKF 1D, and
690 precipitation are also provided. The trends in the TWSV, SMSV and GWSV for the 4 basins,
691 as well as the areally-averaged values for the entire Hexi Corridor, are given in Table 7. The
692 average EnKF 3D trends are all negative: approximately -0.2, -0.1, and -0.1 cm/yr for
693 TWSV, SMSV, and GWSV, respectively. This reduction in the water storages is observed
694 despite the increased amount of rainfall, which shows a positive trend of about 0.4
695 (mm/month)/yr. The water storage reductions can likely be attributed to the extraction of
696 groundwater to meet irrigation demands. In Sect. 6.6, it will be shown that groundwater
697 extractions are essential for that purpose in the Hexi Corridor.

698 Focusing on individual river basins provides additional insight into the water storage issue, as
699 the influence of the large desert area is removed. The water storage losses in the individual
700 basins outside the desert are even more pronounced, particularly in the Shiyang River Basin.
701 This basin had the greatest TWS loss (approximately 0.4 cm/yr), which was entirely caused
702 by the reduction of GWS. This can be explained by groundwater abstraction to meet the
703 irrigation demand in the region. The Heihe and Shule River Basins also experienced a TWS
704 loss of ~0.2 cm/yr, which came from a reduction of both soil moisture and groundwater
705 storages. Again, the negative GWS trend was likely caused by significant pumping of

706 groundwater to maintain crop production. This is consistent with the extreme water stress
707 over the Heihe River basin between 2001 and 2010, which was documented in Table 11.7 of
708 the study by Chen et al. (2014). In the Desert Region, in contrast to other basins, the minor
709 decreasing TWS trend of -0.1 cm/yr was dominated by loss of SM storage. This was likely
710 caused by inaccurate model parameter calibration over the Desert Region (i.e., too large SC
711 value). Separation of the TWS into groundwater and soil moisture store was likely incorrect.
712 As such, the annual signal in GWS is much less than in SM there. Therefore, GRACE update
713 was mostly attributed to the SM component, so that a groundwater-pumping signature (Jiao et
714 al., 2015) was seen in the SM instead of the GWS layer.

715

716 **6.6 Connection to agriculture activity**

717 Figure 15 shows the monthly averaged groundwater head measurements at wells W1 to W5 in
718 the Shiyang River Basin (Fig. 1c). Monthly averaged precipitation and NDVI values are
719 shown as well. Since extracted water can be used to support agriculture not only at the well
720 location but also in the nearby area, precipitation and NDVI are reported as the average values
721 within a circular area of the 10-km radius. These data will be used to ascertain if groundwater
722 extractions to support agriculture might be the source of the negative GWS trends observed in
723 Fig. 12 and Table 6. From Fig. 14, it is noticed that the growing period is approximately
724 between May and October, where the amount of rainfall is higher than 15 mm/month and the
725 NDVI is typically greater than 0.2. By observing well measurements, precipitation, and NDVI
726 together, some groundwater extraction signatures can be explained by the extension of the
727 growing period over the dry season. For example, at station W1, the groundwater in 2010 was
728 lower than the average, showing a gradual decrease in summer (Fig. 15a). One may attribute
729 this to the shortage of rainfall in July and August 2010, which was lower than the average
730 (Fig. 15b). However, the NDVI value was higher than the average during summer 2010 (Fig.
731 15c), which implies that water from other sources than precipitation was probably used to
732 maintain the growing period. This additional water was likely extracted from the ground, and
733 such an activity led to a decreased groundwater table during summer 2010. A similar
734 explanation can be applied to station W2, where low groundwater head, low rainfall, and high
735 NDVI were observed in summer 2007 and summer 2008 (Fig. 15 d,e,f). At station W3, the
736 behaviour is similar to station W1: the extension of the growing period was observed in
737 summer 2010, where the GWS and precipitation were lower than the average, while NDVI
738 was significantly higher (Fig. 15 g,h,i). Groundwater pumping signatures were not present at
739 stations W4 and W5.

740

741 **7. Conclusions**

742 This study was focused on the estimation of water resources dynamics in the Hexi Corridor by
743 assimilating GRACE-derived TWSV into the PCR-GLOBWB hydrological model. Validating
744 against well data showed that DA led to noticeable improvement in the state estimates in
745 terms of correlation, RMSD, and long-term trend. Furthermore, GRACE DA estimates

746 revealed the reduction of water storages between 2002 and 2010. The Shiyang River Basin –
747 the southeaster part of the Hexi Corridor area – suffered the most from the water loss, which
748 was likely caused by the overuse of the groundwater for irrigation. Due to inaccurate
749 groundwater abstraction information, PCR-GLOBWB alone could not properly capture the
750 downward trend of water storages. This highlights the value of the GRACE DA in this
751 situation. It should be emphasized that GRACE does not fix a technical problem of the
752 hydrological model, but rather it provides information, which is not available otherwise. Note
753 that, in principle, the model may predict any long-term behaviour of water storage, but that
754 information should be brought in "by hand" (e.g., via the groundwater abstraction parameter).
755 As soon as that information is not available, reliable long-term predictions on the basis of
756 hydrological modelling alone are conceptually impossible. GRACE DA acts as a provider of a
757 missing puzzle piece here. Of course, the performance of GRACE DA needs to be further
758 investigated in other geographical locations and with different hydrological models to confirm
759 its benefits.

760 A substantial decrease in the water storage in the Hexi Corridor between 2002 and 2010,
761 particularly over the Shiyang River Basin, took place in spite of the increased precipitation.
762 The amount of water from rainfall was likely insufficient to support irrigation water
763 requirements. Irrigation water demands increased significantly to maintain the crop
764 production and, as a result, the region was under extreme water stress. Water consumption
765 from all available sources was essential for bridging the deficit, including a sizeable amount
766 of groundwater extraction. This study illustrates how ground observations and remote sensing
767 data may reveal the connection between groundwater pumping and agricultural activity.

768 The conversion approach between the groundwater head measurement and groundwater
769 storage is proven feasible over the Shiyang River Basin. The scale factor estimates produced
770 with this approach are consistent with the specific yield estimated from the field observations.
771 However, it is noted here that the results of the conducted validation might be over-optimistic,
772 since the well data processed with the adopted conversion procedure are not fully independent
773 of the assimilated GRACE data. The specific yield from the field observation must be used
774 when available.

775 Furthermore, we demonstrate how the error covariance matrix **R** of GRACE-derived TWSV
776 can be obtained from the error covariance matrix of GRACE SHCs (which is currently
777 provided together with the SHCs themselves). This study shows that it is necessary to use the
778 **R** matrix in order to properly take into account the error correlations in the DA scheme. To
779 come to that conclusion, we considered 2 variants of the error variance-covariance matrix in
780 the data assimilation: excluding and including error correlations. Validating against well data
781 showed that ignoring error correlations in DA tended to over-fit results to the observations,
782 and in many cases led to less accurate state estimates. This finding is in agreement with the
783 recommendation in Schumacher et al. (2016). We explain this finding by the fact that
784 GRACE errors at the neighbouring $0.5^\circ \times 0.5^\circ$ grid cells are highly correlated. As such, the
785 simultaneous consideration of GRACE data at multiple neighbouring cells does not reduce
786 data noise, as it would be the case if noise were white. In other words, the white-noise
787 assumption may severely overestimate the information content of GRACE data. We recognize

788 that the derivation of GRACE-derived TWSV error variance-covariance matrices is very
789 computationally demanding. Still, we believe that this is a reasonable price to pay as deriving
790 the error variance-covariance matrix from the full (and only full) error covariance matrix
791 noticeably improves the results of GRACE data assimilation.

792 To further improve the DA performance, an extended or an alternative DA framework can be
793 considered. One of the points of attention is only a minor improvement in streamflow
794 estimates, which is caused by an insufficient temporal and spatial resolution of GRACE data.
795 A promising way to go is to improve the runoff scheme at a conceptual level, e.g., by
796 extending GRACE DA with a simultaneous parameter calibration. To that end, the state
797 vector should be extended to also include selected model parameters (Eicker et al., 2014;
798 Wanders et al., 2014). This allows for the adjustment of the storage size and might lead to a
799 more accurate estimate of model states, including streamflow (Wanders et al., 2014).
800 Alternative ensemble-based DA approaches, such as particle filters (Weerts and El Serafy,
801 2006), can also be considered. Particle filters estimate a sample from the realistic posteriori
802 distribution, which is not necessarily Gaussian, like in the EnKF. The approach has been
803 shown very effective for the parameter calibration (Dong et al., 2015).

804 Finally, the usage of improved gravity solutions to be available after the launch of the
805 GRACE Follow-on mission (Flechtner et al., 2014) will probably further increase the
806 accuracy of the GRACE DA estimates.

807

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819

820 **8. References**

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1055 **Table 1.** PCR-GLOBWB model parameters related to the TWS estimate. Parameters are
 1056 functions of spatial coordinates, except DDF which is a constant.

Parameter	Description	unit
$K_{\text{sat,up}}$	Saturated hydraulic conductivity of the upper soil storage	m/day
$K_{\text{sat,low}}$	Saturated hydraulic conductivity of the lower soil storage	m/day
SC_{up}	Storage capacity of the upper soil	m
SC_{low}	Storage capacity of the lower soil	m
$f_g^{\min}, f_f^{\min}, f_p^{\min}, f_{np}^{\min}$	Minimum soil depth fraction of grassland (g), forest (f), paddy irrigation (p), non-paddy irrigation (np)	-
$f_g^{\max}, f_f^{\max}, f_p^{\max}, f_{np}^{\max}$	Maximum soil depth fraction of grassland (g), forest (f), paddy irrigation (p), non-paddy irrigation (np)	-
J	Groundwater recession coefficient	1/day
DDF	Degree-day factor in the snow pack	°Cm/day
KC^{\min}	Minimum crop coefficient	-

1057

1058 **Table 2.** TWSV, SMSV and GWSV estimated annual amplitude (A, cm) and phase (P, cm)
 1059 month) in 4 different basins computed between April 2002 and December 2010. Areally
 1060 averaged values for the entire Hexi Corridor are also given.

		Shiyan	Heihe	Desert	Shule	Areally-average
TWSV	GRACE	A 2.05 ± 0.31 P 6.97 ± 0.29	1.49 ± 0.21 6.80 ± 0.27	1.79 ± 0.23 6.49 ± 0.24	1.21 ± 0.27 8.61 ± 0.42	1.43 ± 0.18 7.05 ± 0.24
	EnOL	A 1.35 ± 0.16 P 6.35 ± 0.23	0.90 ± 0.07 5.61 ± 0.14	0.66 ± 0.07 5.80 ± 0.19	0.37 ± 0.06 5.40 ± 0.31	0.70 ± 0.06 5.74 ± 0.16
	EnKF 1D	A 1.61 ± 0.16 P 6.96 ± 0.19	0.87 ± 0.10 6.80 ± 0.22	1.05 ± 0.11 6.47 ± 0.19	0.40 ± 0.11 8.35 ± 0.51	0.80 ± 0.09 6.92 ± 0.23
	EnKF 3D	A 1.49 ± 0.13 P 6.42 ± 0.17	0.80 ± 0.08 6.12 ± 0.19	0.72 ± 0.07 6.40 ± 0.20	0.26 ± 0.09 8.48 ± 1.02	0.72 ± 0.07 6.44 ± 0.22
SMSV	EnOL	A 1.03 ± 0.11 P 5.77 ± 0.20	0.70 ± 0.06 5.60 ± 0.16	0.62 ± 0.07 5.82 ± 0.21	0.31 ± 0.05 5.03 ± 0.32	0.59 ± 0.06 5.62 ± 0.18
	EnKF 1D	A 0.88 ± 0.09 P 6.55 ± 0.21	0.75 ± 0.09 7.01 ± 0.22	0.99 ± 0.11 7.08 ± 0.21	0.36 ± 0.10 8.47 ± 0.54	0.67 ± 0.08 7.26 ± 0.24
	EnKF 3D	A 1.30 ± 0.10 P 5.59 ± 0.15	0.66 ± 0.07 6.25 ± 0.20	0.71 ± 0.08 6.44 ± 0.20	0.12 ± 0.08 8.19 ± 0.37	0.55 ± 0.07 6.32 ± 0.22
GWSV	EnOL	A 0.50 ± 0.08 P 7.84 ± 0.29	0.19 ± 0.03 7.13 ± 0.26	0.02 ± 0.004 5.43 ± 0.34	0.09 ± 0.01 6.91 ± 0.29	0.12 ± 0.01 7.22 ± 0.21
	EnKF 1D	A 0.65 ± 0.05 P 8.69 ± 0.16	0.12 ± 0.03 7.82 ± 0.40	0.01 ± 0.01 7.91 ± 1.90	0.05 ± 0.01 8.49 ± 0.29	0.10 ± 0.01 8.32 ± 0.25
	EnKF 3D	A 0.70 ± 0.06 P 8.52 ± 0.16	0.11 ± 0.02 7.50 ± 0.31	0.02 ± 0.01 7.76 ± 1.00	0.05 ± 0.01 8.66 ± 1.33	0.10 ± 0.01 8.26 ± 0.23

1061

1062 **Table 3.** Averaged values and standard deviations of precipitation and model parameters for 4
 1063 different basins.

	Shiyan	Heihe	Desert	Shule
Precipitation (mm/month)	21 ± 12	13 ± 12	11 ± 2	8 ± 6
$SC_{\text{up}} (\text{m})$	0.08 ± 0.02	0.09 ± 0.02	0.09 ± 0.01	0.08 ± 0.01
$SC_{\text{low}} (\text{m})$	0.33 ± 0.08	0.37 ± 0.07	0.35 ± 0.04	0.33 ± 0.08

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1066 **Table 4.** Statistical values of the GWSV computed from the in situ well measurement and
 1067 GRACE DA estimates between January 2007 and December 2010. The average values are
 1068 computed by averaging the estimated statistical values from all well locations.

		W1	W2	W3	W4	W5	Average value
Correlation coefficient [-]	EnOL	0.74	0.17	-0.04	-0.05	-0.53	0.06
	EnKF 1D	0.84	0.32	0.90	0.45	0.64	0.63
	EnKF 3D	0.82	0.49	0.85	0.51	0.83	0.70
RMS difference [cm]	EnOL	0.69	1.67	0.77	3.34	3.81	2.06
	EnKF 1D	0.58	1.63	0.40	2.56	2.58	1.55
	EnKF 3D	0.63	1.43	0.38	2.24	1.27	1.19

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1070 **Table 5.** Long-term trends and standard deviations of the in situ data and the DA estimates.
 1071 The RMS difference (RMSD) between the in situ data and the DA trend estimates are also
 1072 provided.

	W1	W2	W3	W4	W5	RMSD
In situ	-0.49 ± 0.03	0.01 ± 0.06	-0.60 ± 0.004	0.56 ± 0.12	-1.40 ± 0.03	0
EnOL	-0.57 ± 0.01	-0.64 ± 0.002	-0.01 ± 0.01	-1.69 ± 0.01	1.29 ± 0.02	1.62
EnKF 1D	-0.52 ± 0.02	-0.58 ± 0.04	-0.74 ± 0.02	-1.33 ± 0.08	-1.99 ± 0.13	0.93
EnKF 3D	-0.83 ± 0.02	-0.51 ± 0.03	-0.38 ± 0.01	-0.44 ± 0.08	-1.18 ± 0.06	0.54

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1074 **Table 6.** Statistical values of the streamflow computed from the river stream gauge
 1075 measurement and GRACE DA estimates between April 2002 and December 2010. The
 1076 average values are calculated by averaging the estimated statistical values from both gauge
 1077 locations.

		G1	G2	Average value
Correlation coefficient [-]	EnOL	0.82	0.76	0.79
	EnKF 1D	0.84	0.77	0.81
	EnKF 3D	0.84	0.78	0.81
NS coefficient [-]	EnOL	0.65	0.56	0.61
	EnKF 1D	0.69	0.57	0.63
	EnKF 3D	0.69	0.57	0.63
RMS difference [cm]	EnOL	5.49	3.09	4.29
	EnKF 1D	5.18	3.08	4.14
	EnKF 3D	5.23	3.04	4.14

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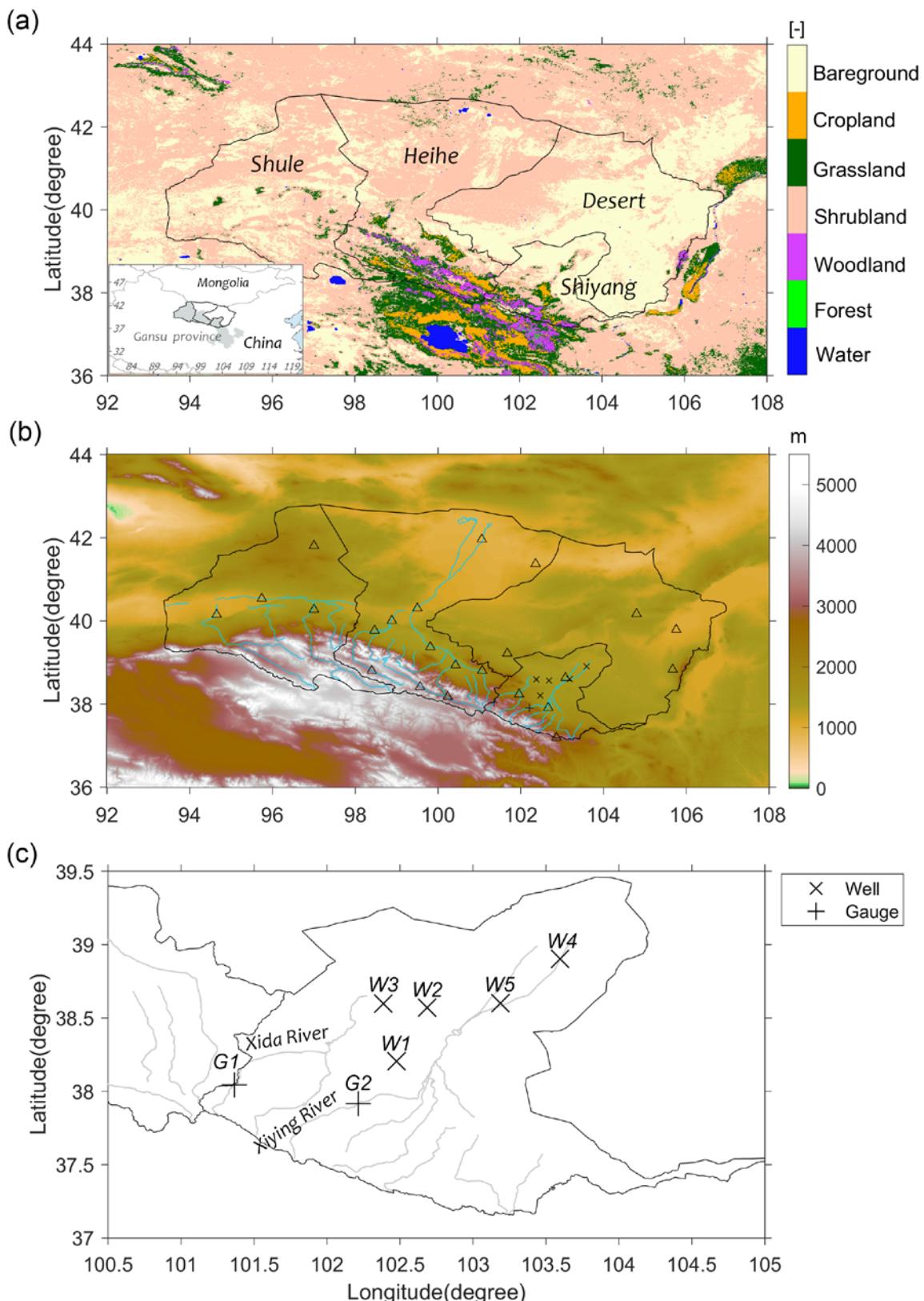
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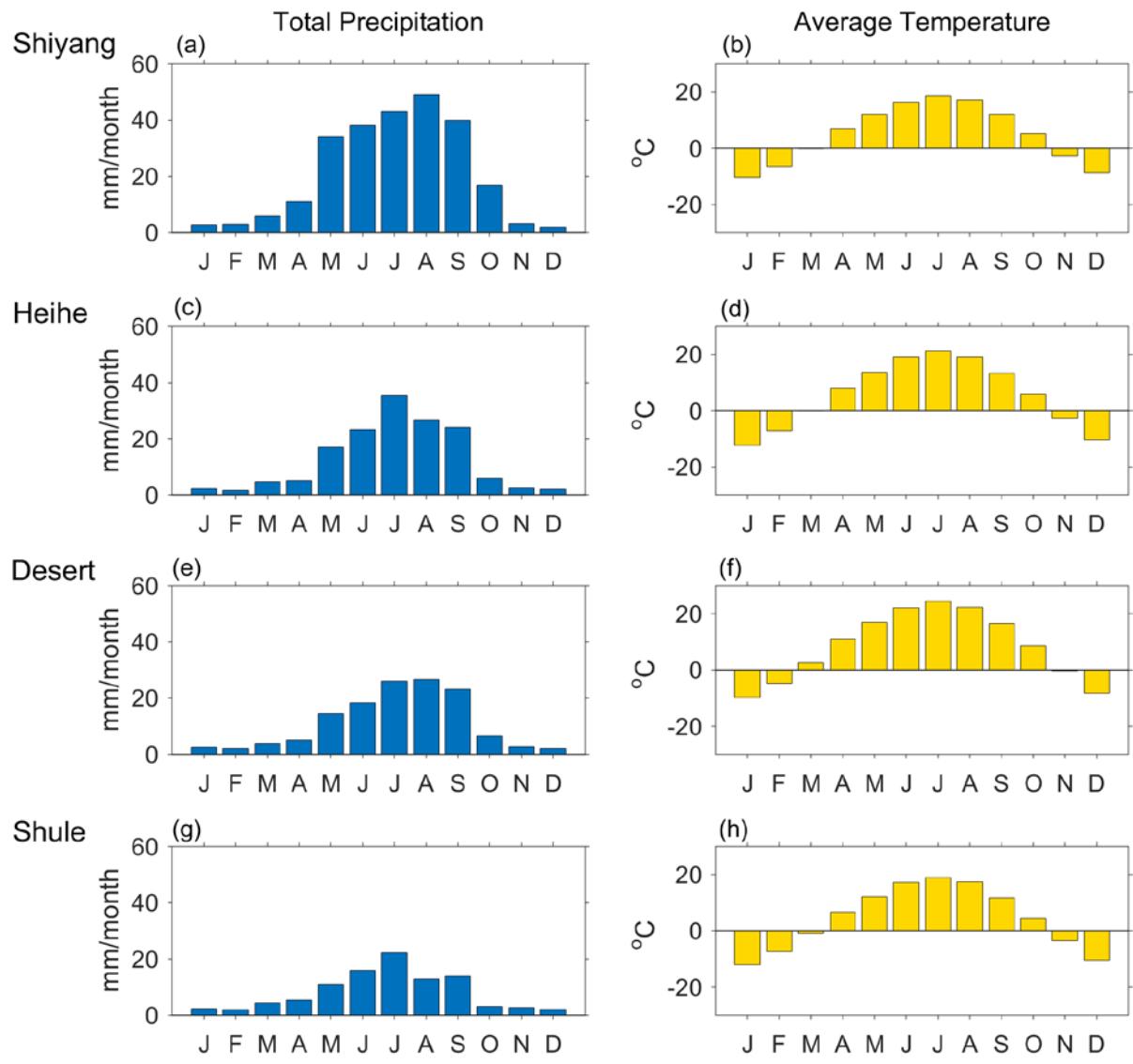
1081 **Table 7.** TWSV, SMSV, GWSV, and precipitation estimated long-term trends in 4 different
 1082 basins computed between April 2002 and December 2010. A really averaged values for the
 1083 entire Hexi Corridor are also given.

		Shiyang	Heihe	Desert	Shule	Areally-average
TWSV (cm/yr)	GRACE	-0.73 ± 0.04	-0.64 ± 0.03	-0.72 ± 0.03	-0.34 ± 0.04	-0.59 ± 0.03
	EnOL	0.30 ± 0.15	0.24 ± 0.09	0.20 ± 0.04	0.18 ± 0.06	0.22 ± 0.07
	EnKF 1D	-0.72 ± 0.08	-0.41 ± 0.04	-0.33 ± 0.05	-0.34 ± 0.04	-0.39 ± 0.07
	EnKF 3D	-0.36 ± 0.02	-0.21 ± 0.02	-0.11 ± 0.03	-0.25 ± 0.03	-0.20 ± 0.03
SMSV (cm/yr)	EnOL	0.38 ± 0.05	0.21 ± 0.02	0.17 ± 0.03	0.14 ± 0.02	0.19 ± 0.02
	EnKF 1D	-0.11 ± 0.03	-0.20 ± 0.01	-0.29 ± 0.04	-0.22 ± 0.04	-0.23 ± 0.03
	EnKF 3D	0.10 ± 0.03	-0.12 ± 0.01	-0.12 ± 0.02	-0.14 ± 0.01	-0.11 ± 0.004
GWSV (cm/yr)	EnOL	-0.08 ± 0.12	0.03 ± 0.07	0.02 ± 0.007	0.04 ± 0.02	0.02 ± 0.04
	EnKF 1D	-0.61 ± 0.01	-0.16 ± 0.004	-0.01 ± 0.005	-0.12 ± 0.02	-0.16 ± 0.02
	EnKF 3D	-0.39 ± 0.01	-0.09 ± 0.003	0.01 ± 0.004	-0.11 ± 0.001	-0.11 ± 0.002
Precipitation ((cm/month)/yr)		0.04 ± 0.01	0.04 ± 0.01	0.05 ± 0.01	0.02 ± 0.01	0.04 ± 0.01

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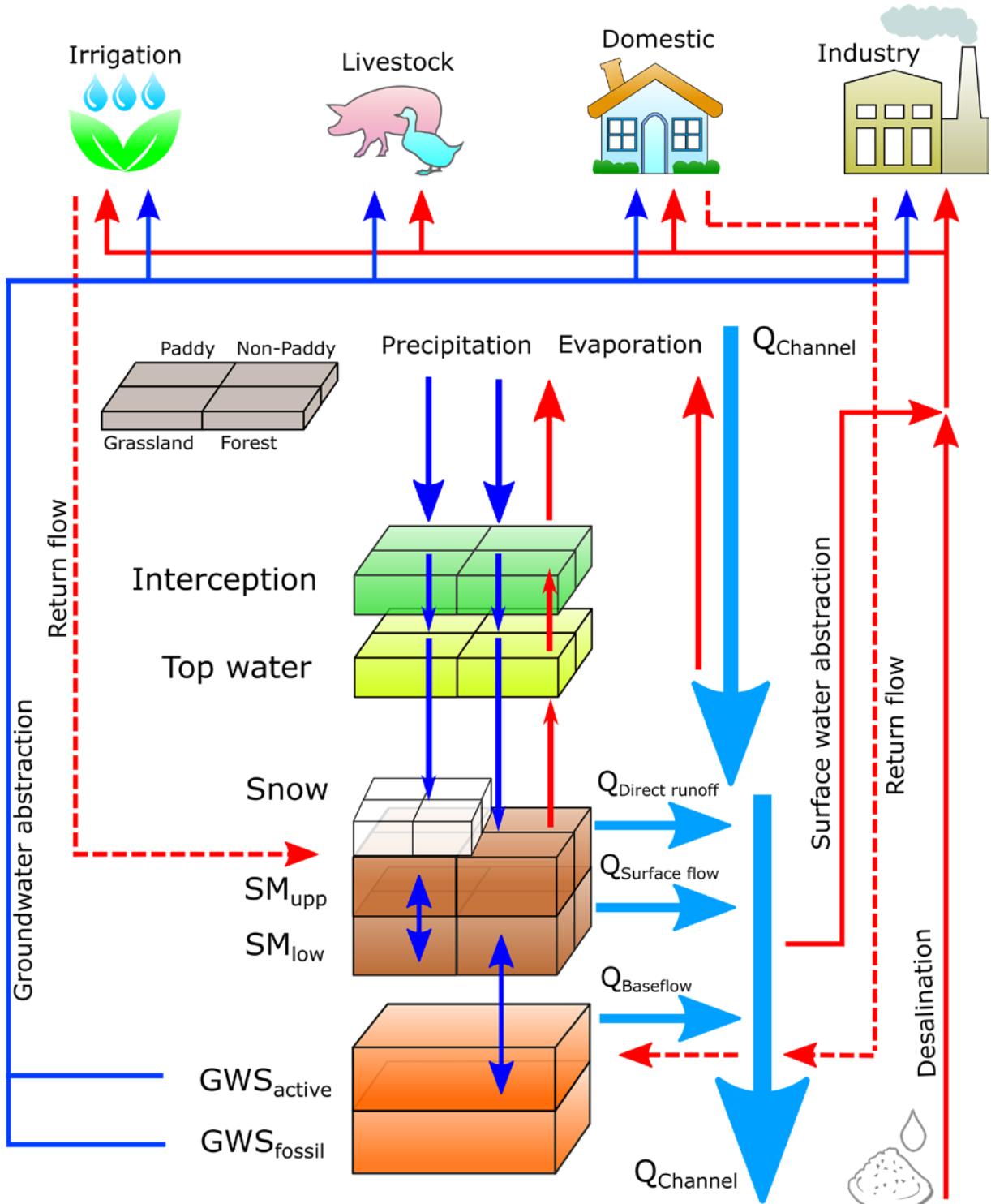
1086 **Figure 1.** Geography of the Hexi Corridor. (a) Land cover and division into individual regions
 1087 (Shiyang River Basin, Heihe River Basin, Shule River Basin, and a Desert), (b) Topography
 1088 and locations of the local meteorological stations (triangles), (c) Zoom-in on the Shiyang
 1089 River Basin, showing the locations of considered groundwater wells (x) and river stream
 1090 gauges (+).



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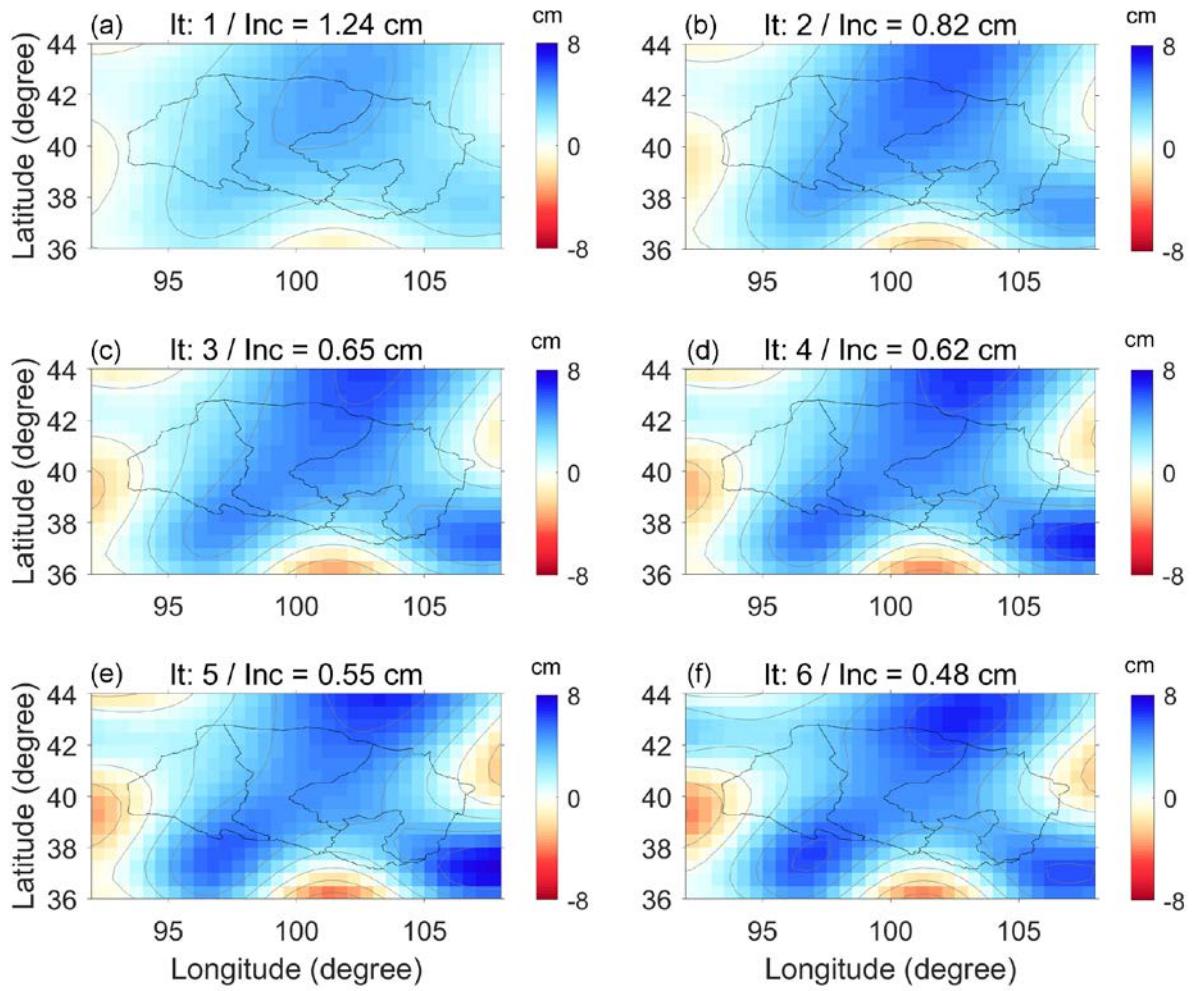
1092 **Figure 2.** Monthly total precipitation and averaged temperature over 4 regions of the Hexi
1093 Corridor.

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1096 **Figure 3.** The structure of PCR-GLOBWB hydrological model.



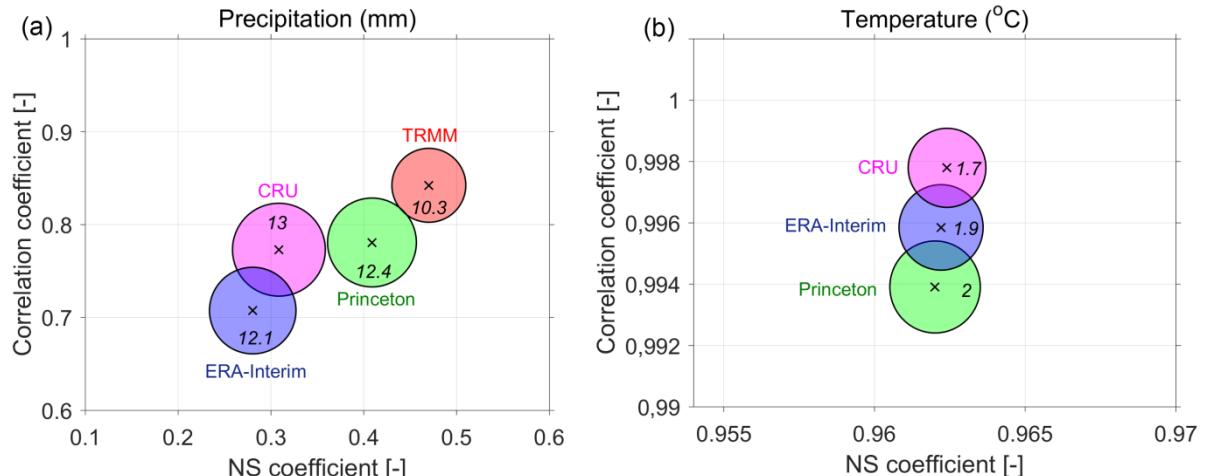
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1098 **Figure 4.** GRACE-derived TWS variation of October 2002. The signal restoration was
 1099 applied to restore the signal mitigated by the applied Gaussian filter. After each iteration (It),
 1100 the increment in each cell was computed. The procedure was stopped after six iterations,
 1101 when the maximum increment (Inc) was lower than 0.5 cm (f).

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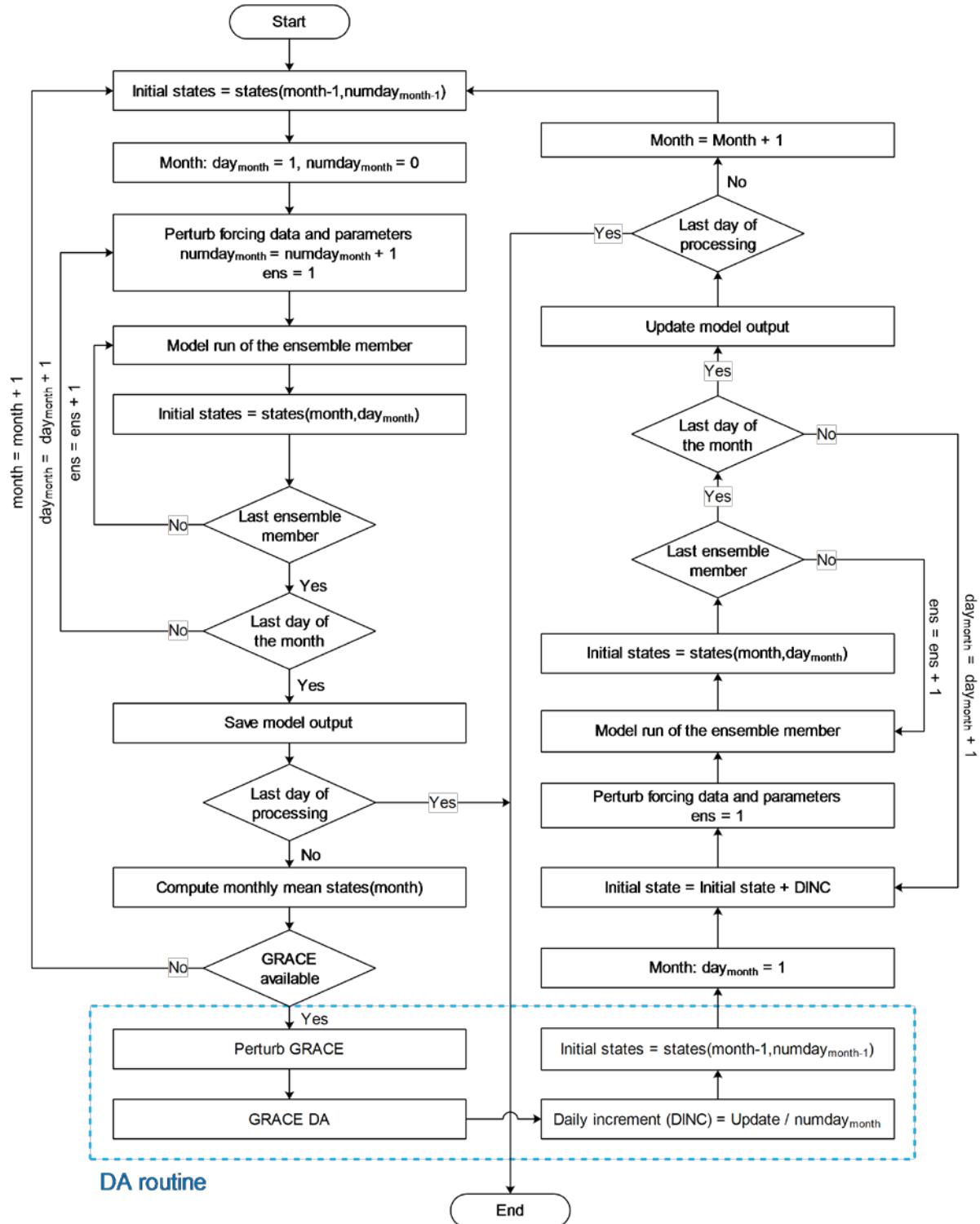
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Figure 5. The correlation coefficient, NS coefficient, and RMS difference computed between the local and different global forcing data. The RMS difference is shown as the radius of the circle (also explicitly provided as the number).

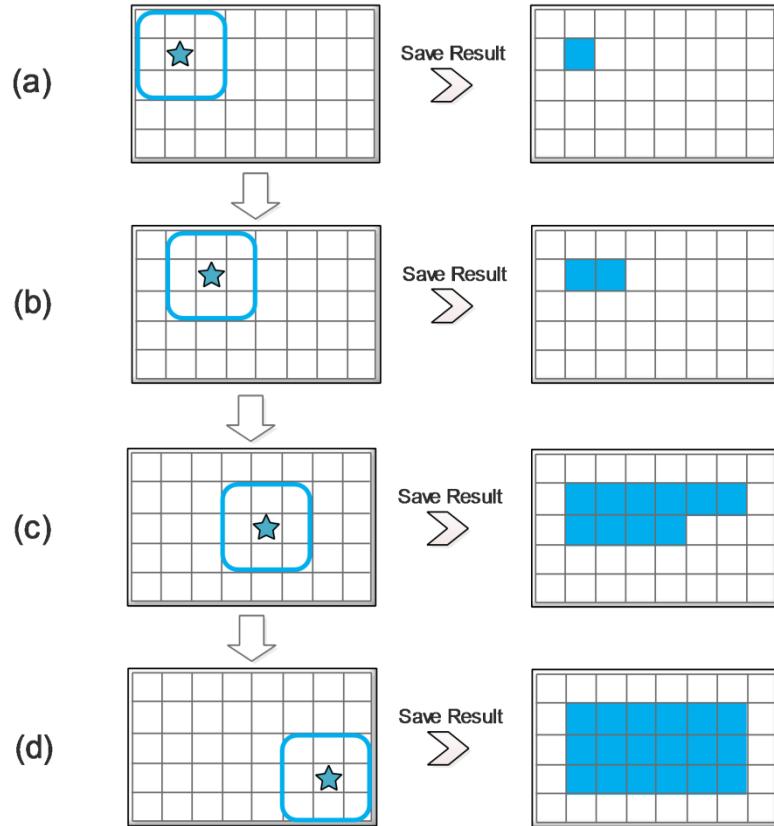
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1111 **Figure 6.** DA diagram representing the disaggregation of monthly averaged TWS from
1112 GRACE into the daily PCR-GLOBWB state estimates.

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1115 **Figure 7.** Demonstration of EnKF 3D scheme, accounting for the spatially-correlated errors.
 1116 For a centre grid cell, the state and observation matrices contain all TWS-related components
 1117 of the neighbouring grid cells and the centre grid cell (left). The graphic demonstrates the case
 1118 of one pixel (0.5 degree) correlation distance. The boundary stretches farther for larger
 1119 correlation distance. The covariance matrices \mathbf{P}_e and \mathbf{R} are computed based on the data from
 1120 these grid cells. Then, the EnKF is applied and the states of the centre grid cell are updated
 1121 (right). The procedure is repeated through all grid cells.

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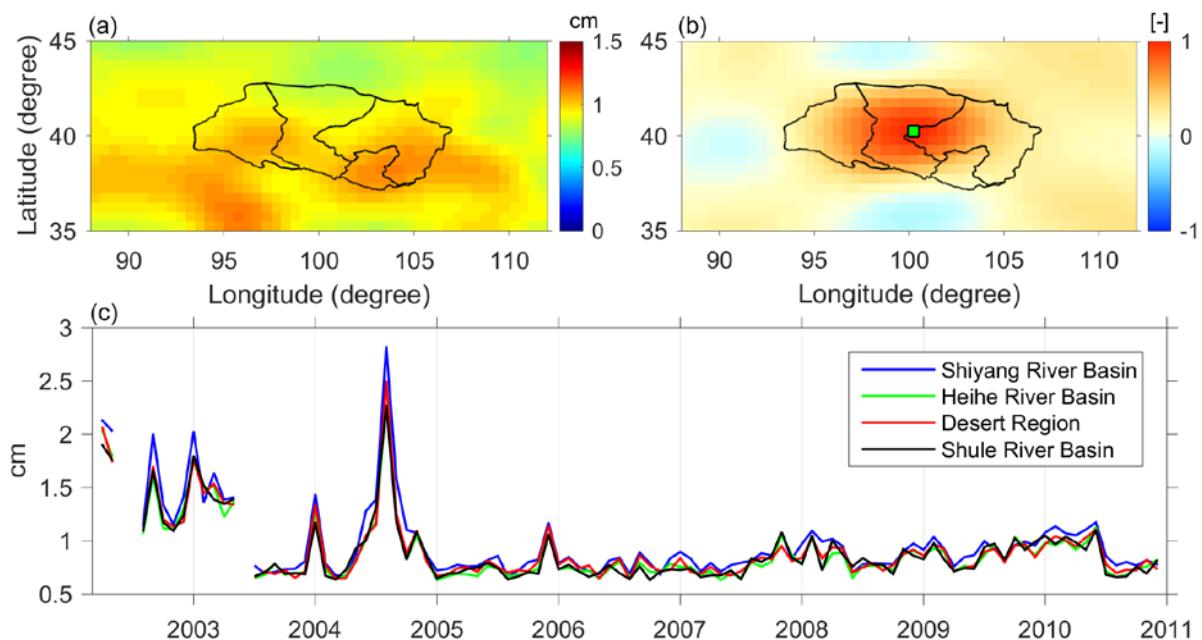
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1134 **Figure 8.** Some statistics of errors in GRACE-derived TWS variation over the Hexi Corridor.
1135 The standard deviation (a) and the correlation coefficient with respect to the green point (b)
1136 for a sample month, October 2002, are shown in the top. The time-series of averaged standard
1137 deviation computed over four different basins are shown in the bottom plot (c).

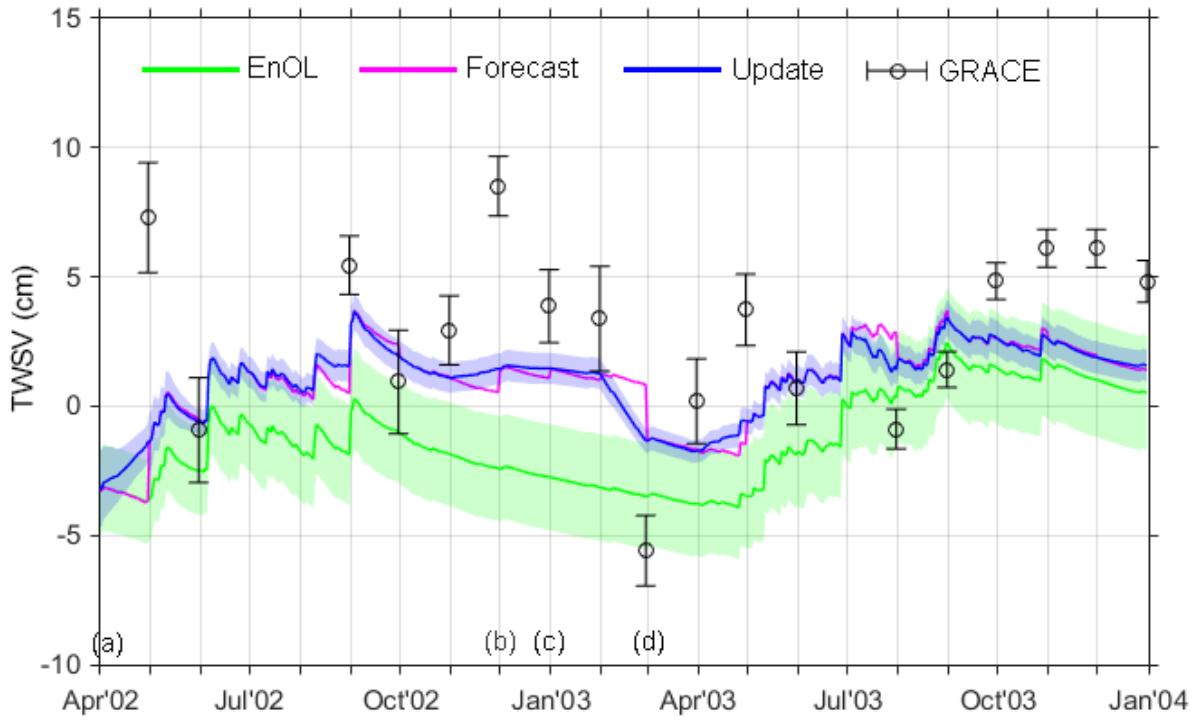
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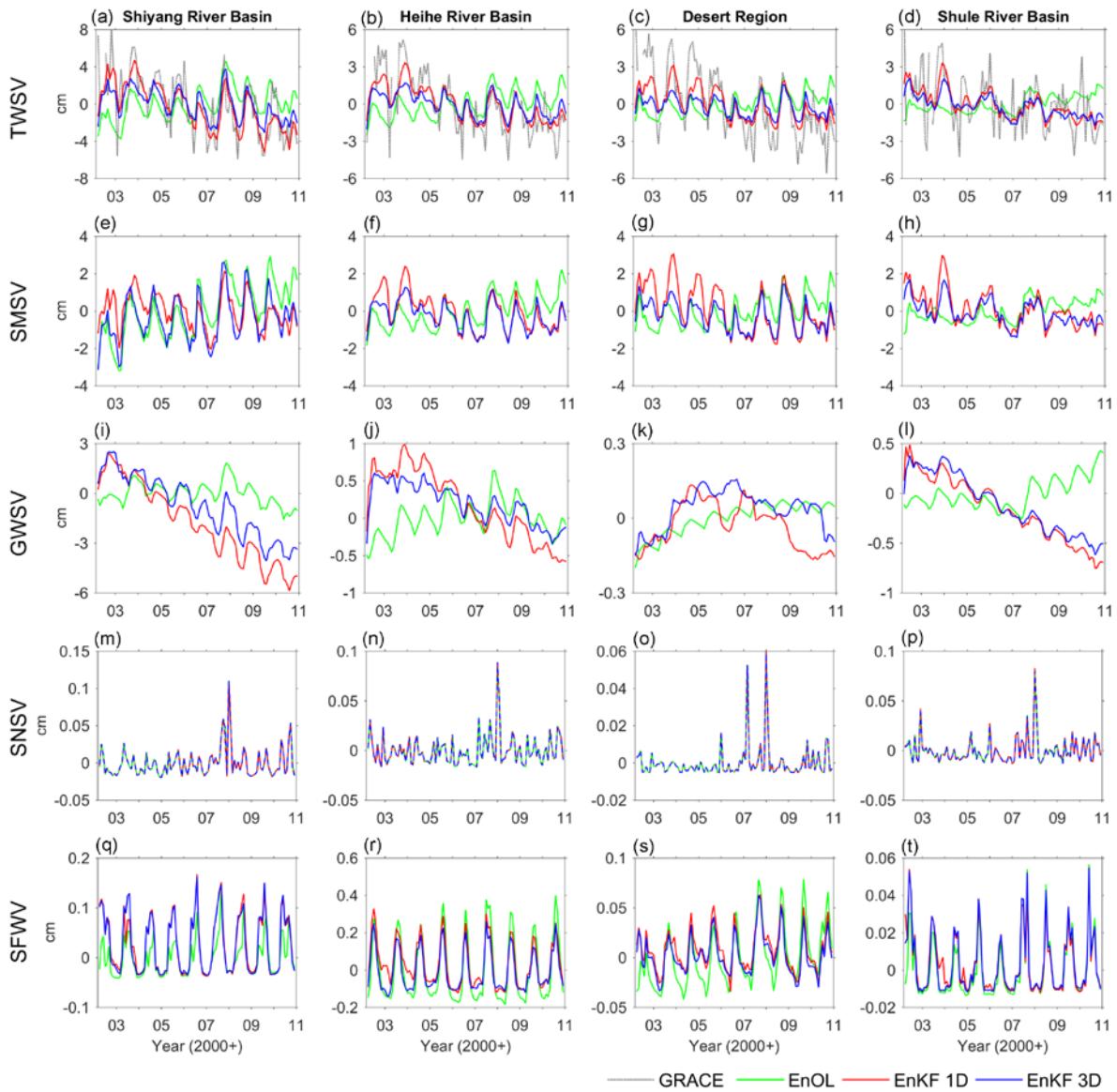
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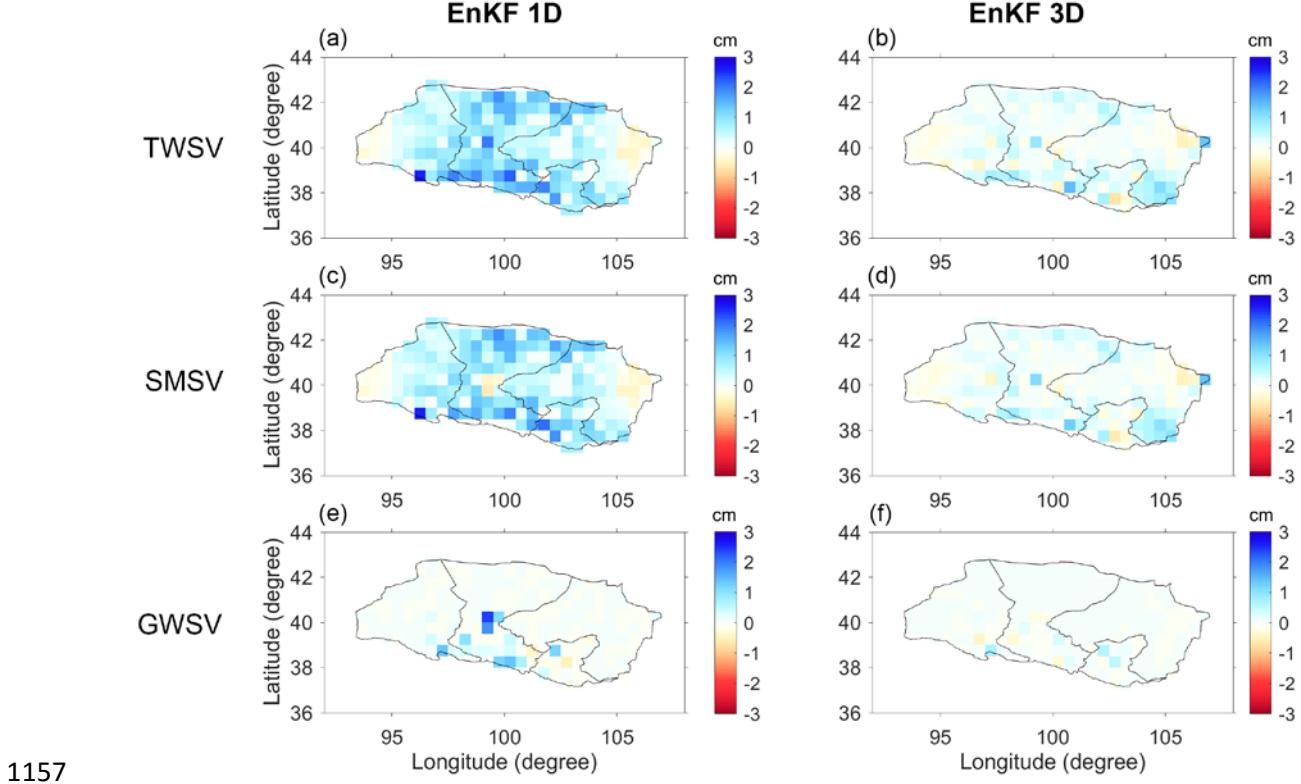
1144 **Figure 9.** Daily TWS variations estimated between 1 April 2002 and 31 December 2003,
 1145 averaged over Shiyang River Basin. The mean value of the ensemble is given as the solid line,
 1146 and the standard deviation is shown as the shaded envelope. The TWS estimates from model
 1147 only (EnOL), GRACE DA forecast (EnKF before the update), GRACE DA update (EnKF
 1148 after update), and GRACE observations are shown. The x-axis labels represent the first day of
 1149 the month. Some features of the DA scheme regarding the identical TWS estimate seen at the
 1150 beginning of the update (point a) and the observed spurious jumps (point b,c,d) are also
 1151 shown.

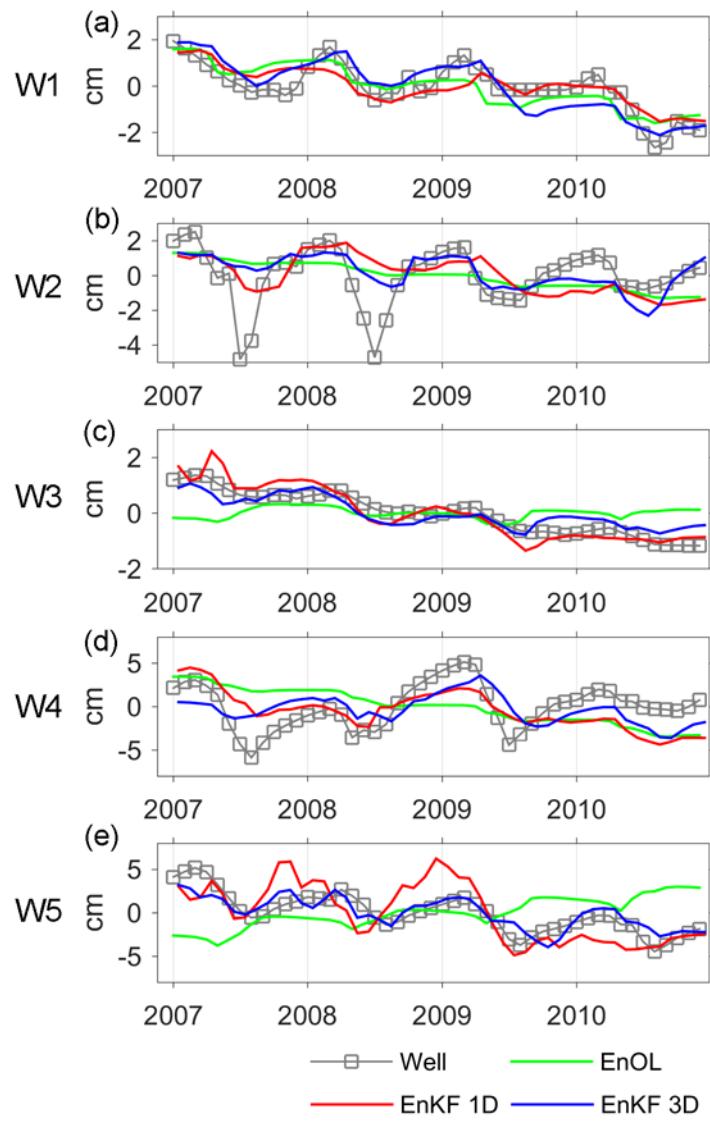
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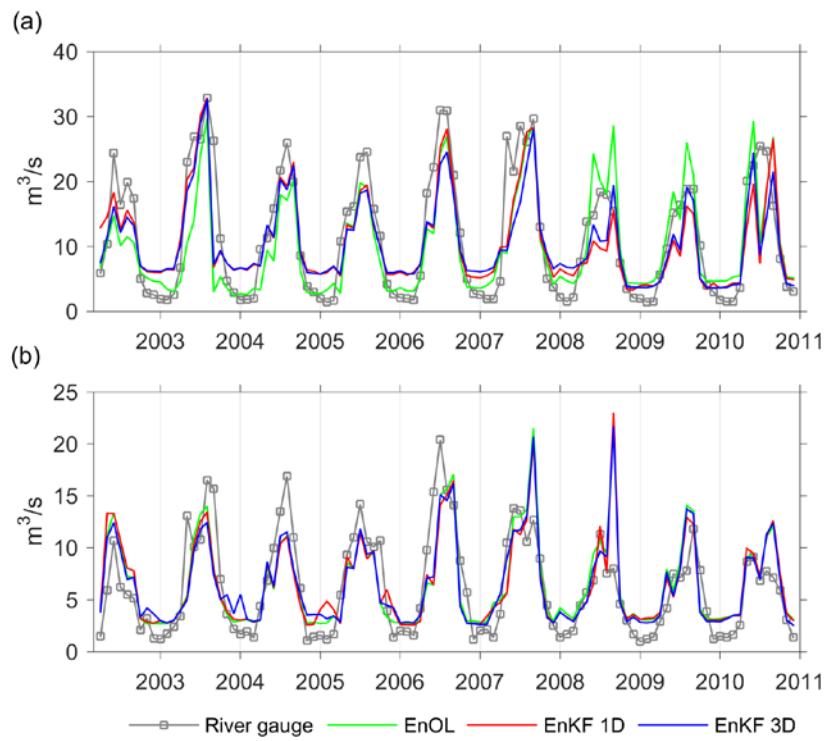
1154 **Figure 10.** Monthly TWSV, SMSV, GWSV, snow water storage variation (SNSV), and
 1155 surface water storage variation (SFWV) estimated between April 2002 and December 2010
 1156 from the EnOL, EnKF 1D, EnKF 3D, and GRACE observations over 4 basins.





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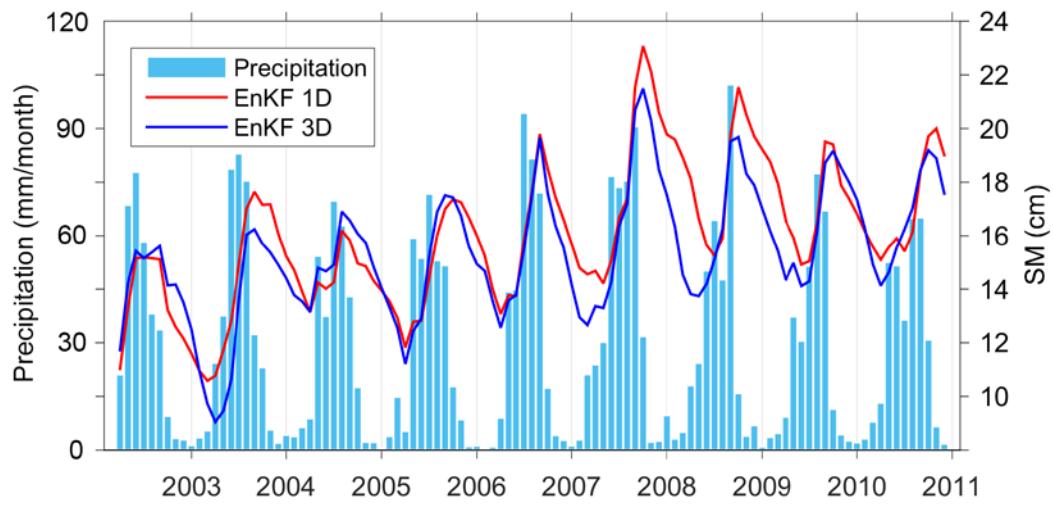
1161 **Figure 12.** Monthly GWS variation estimates from the in situ well measurements, as well as
 1162 EnOL, EnKF 1D, and EnKF 3D results, between January 2007 and December 2010 at 5
 1163 groundwater well locations. The chosen period is based on the availability of the well data.



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1165 **Figure 13.** Monthly streamflow estimates from the in situ river gauge measurements, as well
 1166 as EnOL, EnKF 1D, and EnKF 3D results, between April 2002 and December 2010 at 2 river
 1167 gauge locations, G1 (a) and G2 (b).

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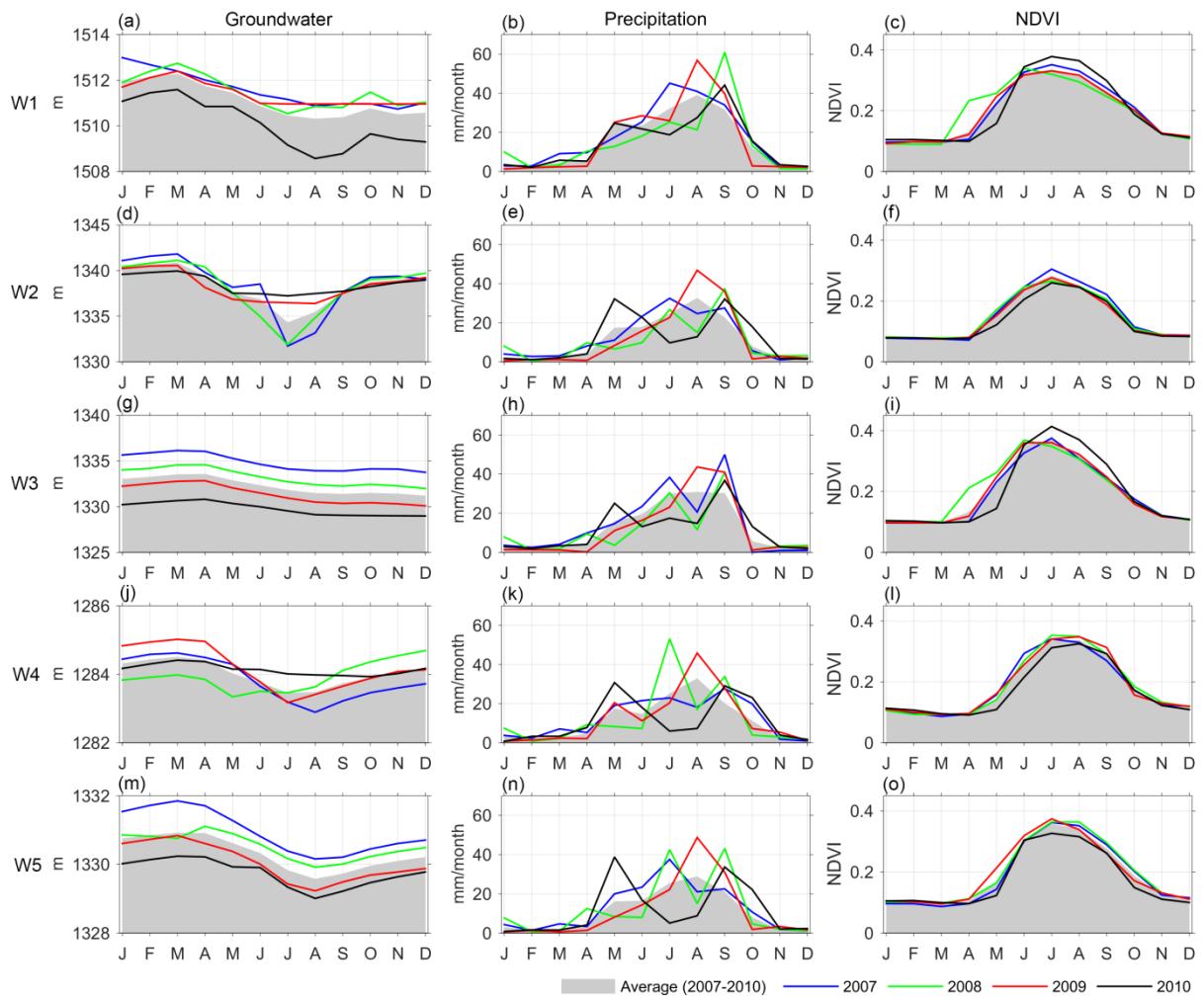
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1170 **Figure 14.** Monthly total precipitation (mm/month) and SM storage estimates (cm) from
 1171 EnKF 1D and EnKF 3D results at river gauge G2 location.

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1176 **Figure 15.** The monthly averaged groundwater head measurement (left)
1177 (middle) and NDVI (right) for five groundwater well locations. Precipitation
1178 and NDVI data are reported as the average values within the circular areas of the 10-km radius. The long-term
1179 average values between January 2007 and December 2010 are shown in the grey shed, and the
1180 values in 2007, 2008, 2009, and 2010 are shown as blue, green, red, and black lines,
1181 respectively. The period is chosen based on the availability of the well data.

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