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1 **Multivariate data assimilation of GRACE, SMOS, SMAP measurements for improved regional**
2 **soil moisture and groundwater storage estimates**

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17

18 **Abstract**

19 Assimilating remote sensing observations into land surface models has become common practice to
20 improve the accuracy of terrestrial water storage (TWS) estimates such as soil moisture and
21 groundwater, for understanding the land surface interaction with the climate system, as well as
22 assessing regional and global water resources. Such remote sensing observations include soil moisture
23 information from the L-band Soil Moisture and Ocean Salinity (SMOS) and Soil Moisture Active
24 Passive (SMAP) missions, and TWS information from the Gravity Recovery And Climate Experiment
25 (GRACE). This study evaluates the benefit of assimilating them into the Community Atmosphere and
26 Biosphere Land Exchange (CABLE) land surface model. The evaluation is conducted in the Goulburn
27 River catchment, South-East Australia, where various in situ soil moisture and groundwater level data
28 are available for validating data assimilation (DA) approaches. It is found that the performance of DA
29 mainly depends on the type of observations that are assimilated. The SMOS/SMAP-only assimilation
30 (SM DA) improves the top soil moisture but degrades the groundwater storage estimates, whereas the
31 GRACE-only assimilation (GRACE DA) improves only the groundwater component. Assimilating
32 both observations (multivariate DA) results in increased accuracy of both soil moisture and
33 groundwater storage estimates. These findings demonstrate the added value of multivariate DA for
34 simultaneously improving different model states, thus leading to a more robust DA system.

35 **Keywords:** SMOS, SMAP, GRACE, EnKS, CABLE, multivariate data assimilation, soil moisture,
36 groundwater

37

38 **1. Introduction**

39 Accurate knowledge on terrestrial water storage (TWS) is crucial for the assessment of climate
40 variation and water resource availability (Entekhabi et al., 1996; Pitman, 2003; Rodell et al., 2007).
41 The accuracy of TWS components (e.g., soil moisture, groundwater, snow, surface water) simulated

42 by land surface models (LSM) at high spatial resolution is commonly degraded by uncertainties in
43 meteorological forcing, model parameter calibration, and land surface process representation
44 (Moradkhani et al., 2005; Wood et al., 2011). Hydrologic information can also be obtained from
45 satellite remote sensing observations (e.g., Kerr et al., 2012; Maurer et al., 2003; Tapley et al., 2004).
46 However, TWS components such as subsurface soil moisture and groundwater are usually not
47 observed directly by in-situ observations, and the limited satellite coverage and sensing depths often
48 restrict the reliability of the observations (Reichle et al., 2008). Data assimilation (DA) can be used to
49 combine various types of observations at different temporal and spatial resolutions with the model
50 simulations according to the relative size of their errors (Reichle, 2008; Reichle et al., 2008). DA has
51 been successfully applied in enhancing model-estimated hydrologic components such as TWS (e.g.,
52 Li et al., 2012), soil moisture (e.g., Lievens et al., 2015), groundwater (e.g., Tangdamrongsub et al.,
53 2018b), snow (e.g., Andreadis and Lettenmaier, 2006), and runoff (e.g., Weerts and El Serafy, 2006).

54 Various satellite observations can be considered in the DA system to improve the key components of
55 the TWS estimate. For example, surface soil moisture has an important role in the variability of the
56 hydrological cycle and climate system (Entekhabi et al., 1996; Koster et al., 2009; Schumann et al.,
57 2009) and can be measured by L-band radiometers, i.e., from the Soil Moisture and Ocean Salinity
58 (SMOS; Kerr et al., 2012) and Soil Moisture Active Passive (Entekhabi et al., 2010) satellite missions
59 (Chan et al., 2016). Both satellite missions provide global soil moisture products at a spatial resolution
60 of ~25 – 36 km (representing the wetness in the top 0 – 5 cm soil layer) approximately every 3 days.
61 The SMOS and SMAP radiometer data have been exploited in soil moisture data assimilation (SM
62 DA) systems over several river basins, e.g., Ahlrigaarde (Western Denmark ; Ridler et al., 2014),
63 Murray-Darling (Lievens et al., 2015), continental Australia (e.g., Tian et al., 2017), the Great Lakes
64 (Xu et al., 2015), and North America (e.g., Blankenship et al., 2016). These studies have
65 demonstrated the benefits of SM DA on both surface and root zone soil moisture components (e.g.,
66 De Lannoy and Reichle, 2016; Tian et al., 2017; Xu et al., 2015). However, SM DA has been found to
67 have a negative impact on the groundwater storage estimate (Tian et al., 2017).

68 In addition to the surface soil moisture, TWS variations (Δ TWS) can be derived from gravity
69 measurements by the Gravity Recovery And Climate Experiment (GRACE) satellite mission (Tapley
70 et al., 2004). The GRACE twin satellites measure changes of the Earth's gravity field every month
71 using a combination of several measurements, including K-band ranging, accelerometer, attitude, and
72 orbital data (Bettadpur, 2012). Because hydrological mass variations are dominant at a monthly time
73 scale, the GRACE data are commonly presented in terms of Δ TWS, and have been used in a wide
74 range of hydrological applications including data assimilation (e.g., Zaitchik et al., 2008; Eicker et al.,
75 2014) for drought detection (e.g., Houborg et al., 2012; Li et al., 2012; Kumar et al., 2016), flood
76 analysis (Reager et al., 2015), groundwater loss analysis (Giroto et al., 2017; Tangdamrongsub et al.,
77 2018b), and snow estimation (Forman et al., 2012; Su et al., 2010). The benefit of GRACE DA was
78 observed particularly in deep storage components such as groundwater storage (e.g., Tangdamrongsub
79 et al., 2015; Zaitchik et al., 2008). However, GRACE DA is generally less effective in surface soil
80 moisture improvement (Li et al., 2012; Tangdamrongsub et al., 2017a; Tian et al., 2017).

81 The goal of multivariate DA is to combine the strengths of SM DA and GRACE DA to
82 simultaneously improve soil moisture and groundwater estimates. Tian et al. (2017) elaborated this
83 concept and showed that the accuracy of surface and deep storage components could be improved by
84 the application of GRACE and SMOS data assimilation. Similarly, Kumar et al. (2018) and Jasinski et
85 al. (2019) applied multivariate DA using multiple satellite soil moisture and snow products to improve
86 the skills of model state estimates and climate assessment indicators. Kumar et al. (2018) showed that
87 the performance of DA is improved with new satellite sensors. Based on these findings, multivariate
88 assimilation of GRACE and L-band satellite soil moisture sensors (e.g., SMOS, SMAP) is expected to
89 lead to increased accuracy of soil moisture and groundwater estimates.

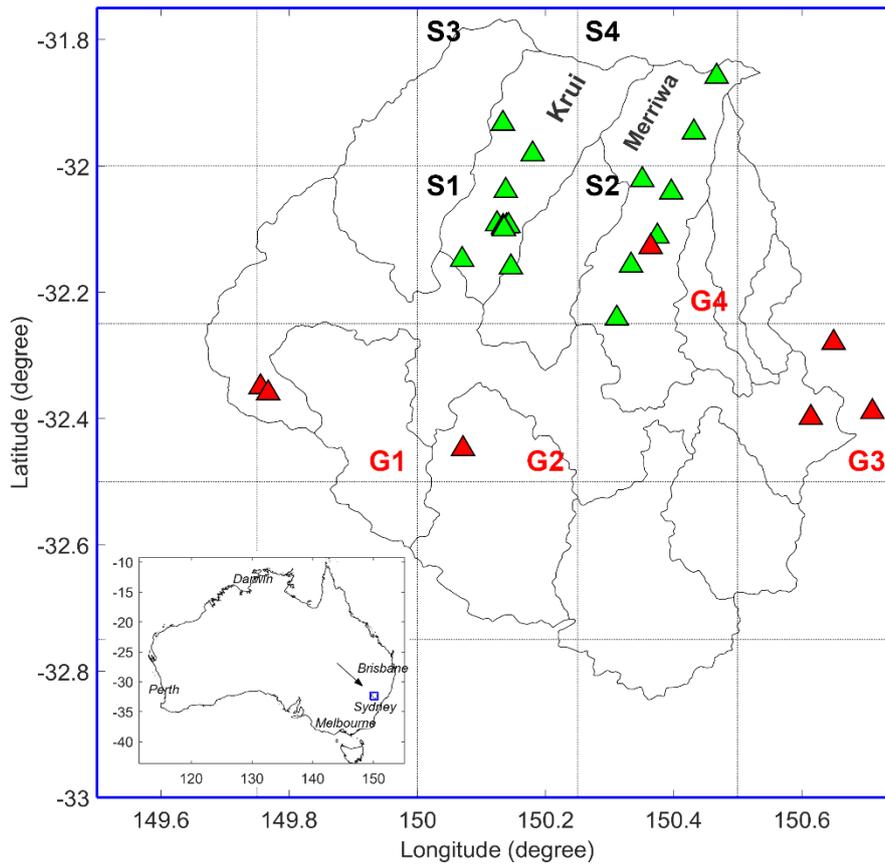
90 This study develops a multivariate DA with GRACE, SMOS, and SMAP data to improve the
91 accuracy of regional soil moisture and groundwater storage estimates. The main research objective is
92 to investigate the performance of multivariate DA in simultaneously improving soil moisture and
93 groundwater storage estimates. Different DA schemes are developed to incorporate different
94 observations into the DA system simultaneously. Three different DA scenarios subject to three
95 different observation cases (SM-only, GRACE-only, and both) are evaluated in terms of estimating
96 water storage (e.g., surface and root zone soil moisture, and groundwater). The DA approach is
97 developed based on ensemble Kalman smoother (EnKS, see, e.g., Dunne et al., 2007; Dong et al.,
98 2015; Tian et al., 2017; Tangdamrongsub et al., 2018b). The LSM used in this study is the
99 Community Atmosphere and Biosphere Land Exchange (CABLE; Decker, 2015). The analysis is
100 conducted over the Goulburn River catchment (Rüdiger et al., 2007) located in the eastern part of
101 New South Wales, Australia, where extensive records of in situ soil moisture and groundwater are
102 available from more than 20 sites throughout the catchment. The DA results are assessed by
103 comparing them against the in situ data, and the ensemble open-loop estimate (EnOL, model run
104 without DA). The evaluation is performed between January 2010 and December 2015, when GRACE,
105 SMOS, SMAP (from March 2015), and in situ data are available.

106

107 **2. Materials**

108 **2.1 Study area**

109 The Goulburn River catchment is located in the south-eastern part of the Murray-Darling basin and
110 has a sub-humid or temperate climate (Fig. 1). The catchment has a total area of 6,540 km² and
111 consists of more than ten sub-catchments, including the Krui and Merriwa catchments where in situ
112 soil moisture data are regularly recorded. The catchment is maintained by the Scaling and
113 Assimilation of Soil Moisture and Streamflow (SASMAS) project (Rüdiger et al., 2007;
114 <http://www.eng.newcastle.edu.au/sasmas/SASMAS/sasdata.html>). The land cover of the catchment
115 consists of a floodplain, clear grassland, crop in the northern part, and a mountain range with dense
116 vegetation in the south. The northern part of the catchment is particularly suitable for satellite soil
117 moisture remote sensing studies due to its low to moderate vegetation cover. Furthermore, the clay
118 content of the top soil layer (0 – 5 cm) in the northern part is several times greater than in the south
119 (Senanayake et al., 2019; <http://www.clw.csiro.au/aclep/soilandlandscapegrid>). Higher variability in
120 the top soil moisture can, therefore, be anticipated in the northern area. The mean annual rainfall of
121 the catchment is ~700 mm and reaches ~1100 mm in the higher altitude areas. Monthly mean
122 minimum/maximum temperatures reach approximately 16°/30° C in summer and 2°/14° C in winter.
123 No snowfall is presented in the catchment. LSM simulations are expected to perform well over the
124 catchment due to the absence of groundwater abstraction and streamflow control.



125

126 **Figure 1.** The geographical location of the Goulburn River catchment, located in South-East Australia
 127 (see the inserted map). The black dotted squares indicate the 25 km model grid cells while the blue
 128 boundary denotes the GRACE grid cell used in this study. The locations of the in situ soil moisture
 129 and groundwater data are shown as green and red triangles, respectively. All in situ soil moisture
 130 data inside the same model grid cell are averaged, resulting in S1 – S4 in situ soil moisture grid cells. A
 131 similar approach is applied to the in situ groundwater data, resulting in G1 – G4 in situ groundwater
 132 grid cells.

133

134 **2.2 Land surface model setup**

135 The Community Atmosphere and Biosphere Land Exchange (CABLE) land surface model is used to
 136 simulate daily volumetric soil moisture and groundwater storage at approximately 25 km resolution
 137 (see Fig. 1). The model can be obtained from <https://trac.nci.org.au/trac/cable>, and the model user
 138 guide and descriptions can be found in Decker (2015), Kowalczyk et al. (2006), and Ukkola et al.
 139 (2016). CABLE estimates soil moisture in six separate layers. In this study, the soil thicknesses from
 140 the top to bottom compartments are set to 1.2, 3.8, 25, 39.9, 107.9, 287.2 cm, respectively. In
 141 comparison with the in situ data (see Sect. 2.5), the combination of the first two model soil layers
 142 represents the 0 – 5 cm soil moisture component while the combination of the first three denotes the 0
 143 – 30 cm component. The forcing data used in CABLE are precipitation, air temperature, snowfall rate,
 144 wind speed, humidity, surface pressure, and shortwave and longwave downward radiation. Similar to
 145 Tangdamrongsub et al. (2018a), the model is forced with meteorological input from the Global Land
 146 Data Assimilation System (GLDAS; Rodell et al., 2004). Following the sensitivity study of
 147 Tangdamrongsub et al. (2018a), GLDAS precipitation is replaced by data from the Tropical Rainfall
 148 Measuring Mission (TRMM; Huffman et al., 2007) to improve the performance of the CABLE model.

149 Two primary error sources of the LSM are the meteorological forcing data and the model parameters.
150 In the DA process (see Sect. 3), the precipitation is perturbed based on the uncertainty provided by the
151 TRMM product (Huffman, 1997). The shortwave radiation is perturbed using multiplicative white
152 noise, with 10% of the nominal values. An additive white noise is used for the air temperature. It is
153 acknowledged that while a homoscedastic error would be more realistic for air temperature, an offline
154 sensitivity analysis found that the temperature error had only a marginal influence on the state
155 estimates compared to e.g. precipitation. The errors of forcing data are assumed to be spatially
156 correlated. As such, an exponential correlation function is applied to the covariance matrix for each
157 forcing variable. The correlation lengths for forcing data were determined using variogram analysis
158 and found to be approximately 25 km. Model parameters associated with soil moisture and
159 groundwater components are also perturbed with a magnitude of 10%. The selected model parameters
160 are the fractions of clay/sand/silt and the drainage parameters that control the soil storage capacity and
161 amount of subsurface runoff, respectively. Both have a direct impact on the soil moisture and
162 groundwater storages (see Table 2 in Tangdamrongsub et al., (2018a) for more details). The
163 perturbation sizes of forcing data and parameters are determined based on the ensemble verification
164 measures (De Lannoy et al., 2006), mainly to allow an adequate spread of the ensemble between
165 updates in the DA process. Table 1 summarizes the forcing and parameter perturbation of this study.
166 Note that the model state is not perturbed directly, but rather perturbed as a result of model
167 propagation associated with the perturbed forcing and perturbed model parameters. As a result, the
168 correlation between soil layers is mainly controlled by LSM physics, and there is no artificially
169 additional imposed error correlation between soil layers.

170 **Table 1.** Perturbations associated with the forcing data and model parameters. The complete
171 parameter description can be found in Decker (2015) and Ukkola et al. (2016).

Forcing/ parameter variables	Description	Spatially correlated	Perturbation type	Standard deviation
Meteorological forcings				
Rainf	Precipitation	Yes	Multiplicative	Obtained from Huffman (1997)
SW	Shortwave radiation	Yes	Multiplicative	10 % of the nominal value
Tair	Air temperature	Yes	Additive	10 % of the nominal value
Model parameters				
$f_{\text{clay}}, f_{\text{sand}}, f_{\text{silt}}$	The fraction of clay, sand, and silt	No	Multiplicative	10 % of the nominal value
f_{sat}	The fraction of the grid cell that is saturated	No	Additive	10 % of the nominal value
q_{sub}	The maximum rate of subsurface drainage assuming a fully saturated soil column	No	Additive	10 % of the nominal value
f_{p}	Tunable parameter controlling drainage speed	No	Additive	10 % of the nominal value

172

173 **2.3 GRACE data processing**

174 The GRACE data release 05 (RL05), provided by the Center for Space Research (CSR), the
175 University of Texas Austin (Bettadpur, 2012), is obtained between January 2010 and December 2015.
176 The product consists of the monthly spherical harmonic coefficient (SHC) complete up to degree and

177 order 96. The full error variance-covariance matrix is also provided as a part of the product. The error
178 matrix is only available up to June 2014, and the monthly average values are used for the missing
179 months (July 2014 – Dec 2015). The GRACE-derived Δ TWS and its uncertainty over the Goulburn
180 catchment are computed following the approach in Tangdamrongsub et al. (2017b). First, the degree 1
181 coefficients (SHC) provided by Swenson et al. (2008) are restored, and the C20 term is replaced by
182 the value estimated from the satellite laser ranging (Cheng and Tapley, 2004). Second, the long-term
183 mean (January 2010 – December 2015) is computed and removed from the monthly product to obtain
184 the SHC variations, and the destriping (Swenson and Wahr, 2006) and 300-km radius Gaussian
185 smoothing filters (Jekeli, 1981) are applied to the SHC variations to suppress the high-frequency
186 noise. Third, the TWS variation (Δ TWS) is computed from the filtered SHC variations using the
187 method described by Wahr et al. (1998). Because the GRACE-derived Δ TWS shows no significant
188 spatial variability over the study area, the catchment averaged Δ TWS is used in this study. Finally, a
189 signal restoration (e.g., Chen et al., 2014) is applied to the computed Δ TWS to restore the damped
190 signal caused by the applied filters. The method iteratively searches for the genuine Δ TWS using a
191 forward model constructed solely from the GRACE data. To be consistent with the model estimate,
192 the temporal mean value of TWS (January 2010 – December 2015) from the CABLE estimate is
193 added to the GRACE-derived Δ TWS to obtain the absolute TWS prior to the assimilation process.
194 Finally, the TWS uncertainty is computed based on the GRACE full error-variance covariance matrix
195 using error propagation (see, e.g., Tangdamrongsub et al. (2017b)). As GRACE error is spatially
196 correlated in nature (Swenson and Wahr, 2006), deriving the error from the available full covariance
197 matrix represents a more realistic GRACE uncertainty compared to the application of a uniform error
198 value (e.g., Tangdamrongsub et al., 2015).

199

200 **2.4 Satellite soil moisture observations**

201 The daily satellite soil moisture retrievals derived from the Soil Moisture and Ocean Salinity (SMOS,
202 Kerr et al., 2012) and the Soil Moisture Active Passive (SMAP, Entekhabi et al., 2010) missions are
203 used in this study. SMOS data are obtained from the level 3 gridded product (Bitar et al., 2017)
204 provided by the Centre Aval de Traitement des Données SMOS (CATDS, <https://www.catds.fr>)
205 operated for the Centre National d'Etudes Spatiales (CNES) by the French Research Institute for
206 Exploitation of the Sea (IFREMER). The data are available from 15 January 2010 to present, with a
207 spatial resolution of ~25 km on the Equal-Area Scalable Earth (EASE; Brodzik et al., 2012) grid. The
208 SMAP data are retrieved from the level 3 (version 4) radiometer global daily 36 km EASE-grid
209 product (SPL3SMP) provided by the National Snow and Ice Data Center Distributed Active Archive
210 Center (NSIDC DAAC, <https://nsidc.org/data/smap>). The product contains the volumetric soil
211 moisture retrieved by the SMAP passive microwave radiometer, available from 31 March 2015 to
212 present. For both SMOS and SMAP, the data are resampled to a 25 km regular grid to reconcile the
213 observations with the model grid space. On days for which more than one SM retrieval is available,
214 the daily average is used to ensure consistency with the model time step.

215 Following previous SM studies (e.g., Colliander et al., 2017; Lievens et al., 2015; Liu et al., 2016), the
216 measurement error of both SMOS and SMAP are both assumed to be $0.04 \text{ m}^3/\text{m}^3$. It is acknowledged
217 that triple collocation analysis (TCA) may potentially provide more accurate SM error estimates
218 (Dong et al., 2018). However, applying TCA in SM DA requires linear consistency between modeled
219 and retrieved SM (Dong et al., 2018). This assumption has not yet been validated in practice.
220 Therefore, constant, rather than TCA-based, error estimates are used in this study.

221 The assimilation of satellite soil moisture data into the LSM requires the application of rescaling to
222 reduce systematic bias that may be found between the model estimate and the observation (Crow et
223 al., 2005; Reichle and Koster, 2004). The bias correction can be used to transform the observation into
224 model space and reduce the inconsistency between their respective climatology (Koster et al., 2009;

225 Renzullo et al., 2014). In this study, cumulative density function matching (CDF-matching; Reichle
 226 and Koster, 2004) is used to rescale satellite observation to LSM climatology. The approach is applied
 227 separately for each model grid cell, and each satellite data product (with respect to its entire period).

228

229 **2.5 In situ data**

230 The in situ soil moisture and groundwater measurements between January 2010 and December 2015
 231 are obtained from the ground observation networks for validation. The in situ soil moisture data are
 232 provided by the SASMAS network (Rüdiger et al., 2007). Data at each depth are provided in terms of
 233 volumetric soil moisture (θ , m^3/m^3). The 0 – 5 ($\theta_{0-5\text{cm}}$) and 0 – 30 cm ($\theta_{0-30\text{cm}}$) data are used in this
 234 study due to their compatibility with the model soil layers (see Sect. 2.2). In situ groundwater level
 235 data (H) are obtained from the Department of Primary Industries (DPI), Office of Water, NSW
 236 (<http://www.water.nsw.gov.au>). Groundwater storage (GWS) simulated in the model can be converted
 237 to H if specific yield data are available. However, this is not the case for the Goulburn Catchment.

238

239 **3. Methodology**

240 **3.1 Ensemble open-loop (EnOL)**

241 The EnOL is used as a reference to evaluate the performance and the uncertainty of the LSM outputs.
 242 In the EnOL, the forcing data (\mathbf{u}) and model parameters ($\boldsymbol{\alpha}$) are perturbed (see Sect. 2.2), and the
 243 model propagation is performed without assimilation as:

$$244 \quad \mathbf{x}_{t|t-1}^i = \mathbf{f}(\mathbf{x}_{t-1}^i, \mathbf{u}_t^i, \boldsymbol{\alpha}^i), \quad (1)$$

245 where \mathbf{f} is the model operator used to propagate the states from $t - 1$ to t , \mathbf{x} is the model state vector,
 246 and $i = 1, 2, 3, \dots, N$ denotes the index of ensemble member (N in total). In this paper, the EnOL
 247 estimate is the ensemble mean of $\mathbf{x}_{t|t-1}^i$. Note that the perturbed initial states are obtained by spinning
 248 up the model (in EnOL mode) for six years (between 2004 and 2009) prior to the assimilation period.
 249 In this study, the state vector (\mathbf{x}) consists of a total of seven variables (soil moisture at six layers and
 250 one groundwater storage, see Sect. 3.2 for more details). The contribution of the snow water and
 251 canopy water components to the total water storage in the Goulburn catchment are negligible. Hence,
 252 they are not included in the state vector. Following Tangdamrongsub et al. (2017a), an ensemble size
 253 of $N = 300$ is used, which is sufficient to ensure the effectiveness of DA in the Goulburn catchment.

254

255 **3.2 Ensemble Kalman smoother (EnKS)**

256 The EnKS consists of a forecast and analysis (update) step. Similar to the EnOL, the states are
 257 propagated forward in time using the LSM in the forecast step. The period of model propagation
 258 depends on the period of the assimilated observations (e.g., approximately one month for GRACE). A
 259 set of observations was computed by perturbing the measurement with its associated covariance \mathbf{R}_s
 260 (Burgers et al., 1998). The subscript s denotes smoother, e.g., $s = t - L + 1 : t$ where L is the
 261 smoother window length. The state vector is updated as:

$$262 \quad \mathbf{x}_{s|s}^i = \mathbf{x}_{s|t-L}^i + \mathbf{K}_s(\mathbf{y}_s^i - \mathbf{H}\mathbf{x}_{s|t-L}^i) \quad (2)$$

263 with

$$264 \quad \mathbf{K}_s = \mathbf{P}_{e,s}\mathbf{H}_s^T(\mathbf{H}_s\mathbf{P}_{e,s}\mathbf{H}_s^T + \mathbf{R}_{e,s})^{-1}, \quad (3)$$

265 where \mathbf{y}_s^i is a perturbed observation vector, \mathbf{H}_s is an operator which relates the ensemble state $\mathbf{x}_{s|t-L}^i$
 266 to the measurement vector \mathbf{y}_s^i , \mathbf{K} is the Kalman gain matrix, and $\mathbf{P}_{e,s}$ and $\mathbf{R}_{e,s}$ are the ensemble error
 267 covariance matrices of the model and observation, respectively. Note that the state variables from $t -$
 268 $L + 1$ to t are considered in the smoother case. If the matrix \mathbf{A} contains the ensemble states and $\bar{\mathbf{A}}$ is
 269 the matrix of the same size as \mathbf{A} and filled with the mean value computed from all ensemble members,
 270 the ensemble error covariance matrix $\mathbf{P}_{e,s}$ can be computed as follows:

$$271 \quad \mathbf{P}_{e,s} = (\mathbf{A} - \bar{\mathbf{A}})(\mathbf{A} - \bar{\mathbf{A}})^T / (N - 1). \quad (4)$$

272 Similarly, \mathbf{R}_e is computed as:

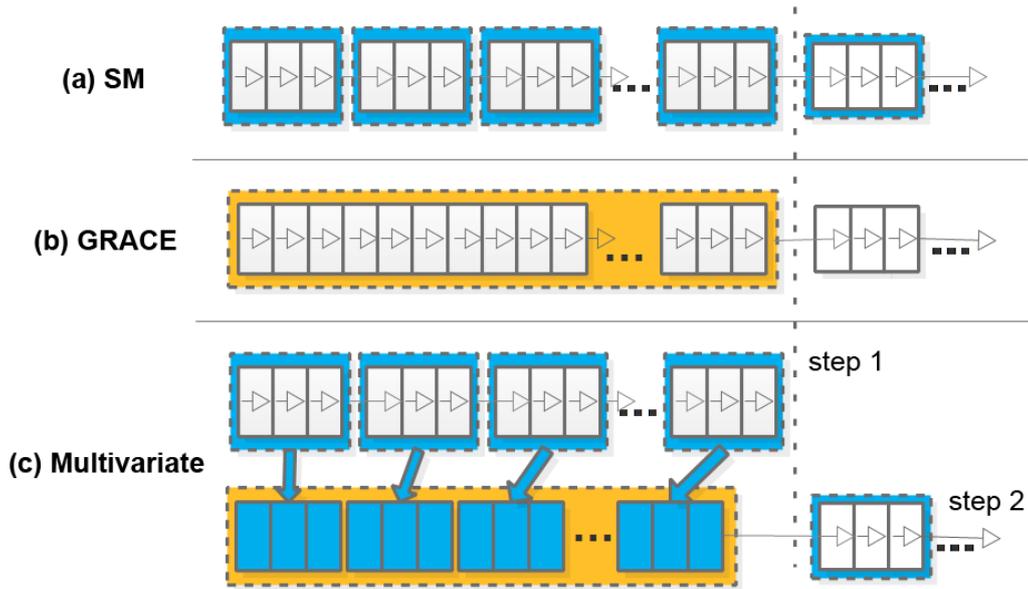
$$273 \quad \mathbf{R}_{e,s} = (\mathbf{D} - \bar{\mathbf{D}})(\mathbf{D} - \bar{\mathbf{D}})^T / (N - 1), \quad (5)$$

274 where \mathbf{D} stores the perturbed observation and $\bar{\mathbf{D}}$ is the ensemble mean. The DA estimate is the
 275 ensemble mean of $\mathbf{x}_{s|s}^i$.

276

277 3.3 Design of the DA schemes

278 The different DA schemes are developed to incorporate observations with different spatial-temporal
 279 resolutions and error characteristics into the DA system simultaneously. Three different DA schemes
 280 are considered here (Fig. 2), SM DA (only soil moisture is assimilated), GRACE DA (only GRACE is
 281 assimilated), and multivariate DA (both soil moisture and GRACE are assimilated).



282

283 **Figure 2.** Three different DA schemes, SM-only DA, GRACE-only DA, and multivariate DA. The
 284 SM DA (a) updates the state estimate using the time window of approximately three days (blue
 285 rectangle in (a)) while the GRACE DA (b) uses the time window of approximately one month (orange
 286 rectangle in (b)). In the multivariate DA (c), the SM DA is first performed (step 1 in (c)), and its
 287 updated states are used as the forecast state in the GRACE DA (step 2 in (c)).

288 As described in Sect. 3.2, the state vector contains daily volumetric soil moisture of six different
 289 layers and groundwater storage components. For a particular model grid cell (j) on a given day (t),
 290 the state vector can be defined as $[\theta_1^{j,t} \ \theta_2^{j,t} \ \theta_3^{j,t} \ \theta_4^{j,t} \ \theta_5^{j,t} \ \theta_6^{j,t} \ gws^{j,t}]^T$, where θ is the volumetric
 291 soil moisture (m^3/m^3), and gws is the groundwater storage (m). The state variables are obtained from
 292 the results of model propagation.

293 In the SM DA (Fig. 2a), the soil moisture observations are assimilated every $L = 3$ days on the model
 294 grid cell individually. Only SMOS data is used between January 2010 and February 2015, and the
 295 dimension of the state vector is $ML \times 1$, where $M=7$ is the number of the state variables. The 3-day
 296 window allows the soil moisture observations to have full coverage over the Goulburn catchment and
 297 yields the adequate ensemble spread between the updates. The observation vector \mathbf{d} contains the
 298 SMOS data with dimension $L \times 1$. The \mathbf{H}_s matrix is defined as:

$$299 \quad \mathbf{H}_s = \begin{bmatrix} \mathbf{h}_{SM}^{j,t=1} & 0 & 0 \\ 0 & \mathbf{h}_{SM}^{j,t=2} & 0 \\ 0 & 0 & \mathbf{h}_{SM}^{j,t=3} \end{bmatrix} \quad (6)$$

$$300 \quad \mathbf{h}_{SM}^{j,t} = [s_1 \quad s_2 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0], \quad (7)$$

301 where s_1, s_2 are the thickness of the first and second soil layers, respectively. The soil thickness is
 302 described in Sect. 2.2. The \mathbf{H}_s matrix (dimension $L \times ML$) relates the SMOS observation to the top two
 303 soil layers. Bias correction is performed prior to the application of DA to reduce the systematic error
 304 between the model estimated and the satellite retrieved soil moisture (see Sect. 3.3). When SMAP
 305 data are available, e.g., from March 2015, the SMOS and SMAP data are assimilated into the LSM,
 306 simultaneously. Lievens et al. (2017) demonstrated that the joint SM DA performed better than a
 307 single SM DA case. In the case of SMOS/SMAP assimilation, the dimension of \mathbf{H}_s and \mathbf{d} are
 308 extended to $2L \times ML$, and $2L \times 1$, respectively, to include the measurement operator associated with the
 309 SMAP data. In this study, the errors in SMOS and SMAP data are assumed to be uncorrelated.

310 In the GRACE DA (Fig. 2b), the model states are updated at a monthly time scale consistent with the
 311 GRACE temporal resolution. The model state vector contains all model grid cells (inside the blue
 312 polygon in Fig. 1) of daily state variables within approximately one month. The state vector is also
 313 constructed from the results of model propagation. The length of the vector is JLM , where J is the
 314 number of grid cells in the study area, and $L \approx 1$ month. The monthly time window used for each
 315 update is based on the time tag of the GRACE product. As the monthly window used to produce a
 316 GRACE solution is not necessarily a calendar month, L is different in each update and varies between
 317 13 and 31 days (following GRACE data used). The observation vector \mathbf{y}_s is a 1×1 vector containing
 318 the monthly average values of the catchment mean TWS. The matrix \mathbf{H}_s is used to convert the
 319 volumetric soil moisture and groundwater storage into the catchment averaged TWS of the month:

$$320 \quad \mathbf{H}_s = [\mathbf{h}_G^{t=1} \quad \mathbf{h}_G^{t=2} \quad \dots \quad \mathbf{h}_G^{t=L}] \quad (8)$$

$$321 \quad \mathbf{h}_G = [\mathbf{g}^{j=1} \quad \mathbf{g}^{j=2} \quad \dots \quad \mathbf{g}^{j=J}] \quad (9)$$

$$322 \quad \mathbf{g}^j = [s_1 \quad s_2 \quad s_3 \quad s_4 \quad s_5 \quad s_6 \quad 1] / JL, \quad (10)$$

323 where $s_1 - s_6$ are the thickness of each soil layer (see Sect. 2.2).

324 In the multivariate DA (Fig. 2c), the SM DA and GRACE DA schemes are combined. The SM DA is
 325 firstly performed (step 1 in Fig. 2c), and its updated state variables are used as the forecast state in the
 326 GRACE DA (step 2).

327 It should be noted that, unlike the 3D EnKF (Reichle et al., 2003), satellite soil moisture observations
 328 are only used for correcting collocated soil moisture estimates. However, a recent study demonstrates
 329 that remote sensing observation error is highly structured in space – suggesting a spatial correlation of
 330 soil moisture retrieval errors (Dong et al., 2017). This complicates the accurate parameterization of
 331 the observation error matrix in a 3D updating DA scheme. Hence, the soil moisture retrievals are not
 332 used for correcting nearby grid cells.

333

334 **3.4 Evaluation metrics**

335 The volumetric soil moisture estimates are validated with the in situ soil moisture and groundwater
336 data in terms of temporal correlation (ρ), and unbiased root mean square difference (ubRMSD;
337 Entekhabi et al., 2010):

$$338 \quad \rho = \frac{\sum(\mathbf{x}_{\text{sim}} - E[\mathbf{x}_{\text{sim}}])(\mathbf{x}_{\text{obs}} - E[\mathbf{x}_{\text{obs}}])}{\sqrt{\sum(\mathbf{x}_{\text{sim}} - E[\mathbf{x}_{\text{sim}}])^2 \sum(\mathbf{x}_{\text{obs}} - E[\mathbf{x}_{\text{obs}}])^2}} \quad (11)$$

$$339 \quad \text{ubRMSD} = \sqrt{E\{[(\mathbf{x}_{\text{sim}} - E[\mathbf{x}_{\text{sim}}]) - (\mathbf{x}_{\text{obs}} - E[\mathbf{x}_{\text{obs}}])]^2\}} \quad (12)$$

340 where \mathbf{x}_{sim} and \mathbf{x}_{obs} are state vectors from simulation (model estimate) and observation (e.g., satellite
341 product, in situ data), respectively, and $E[\cdot]$ is the expectation operator.

342 All in situ soil moisture and groundwater data inside the same model grid cell (Fig. 1) are averaged
343 before the comparison. This produces four grid cells of in situ soil moisture (S1 – S4) and four of in
344 situ groundwater data (G1 – G4). Note that, only the temporal correlation between H and GWS is
345 used to evaluate the groundwater storage estimate (against groundwater level) due to the absence of
346 accurate information on specific yield.

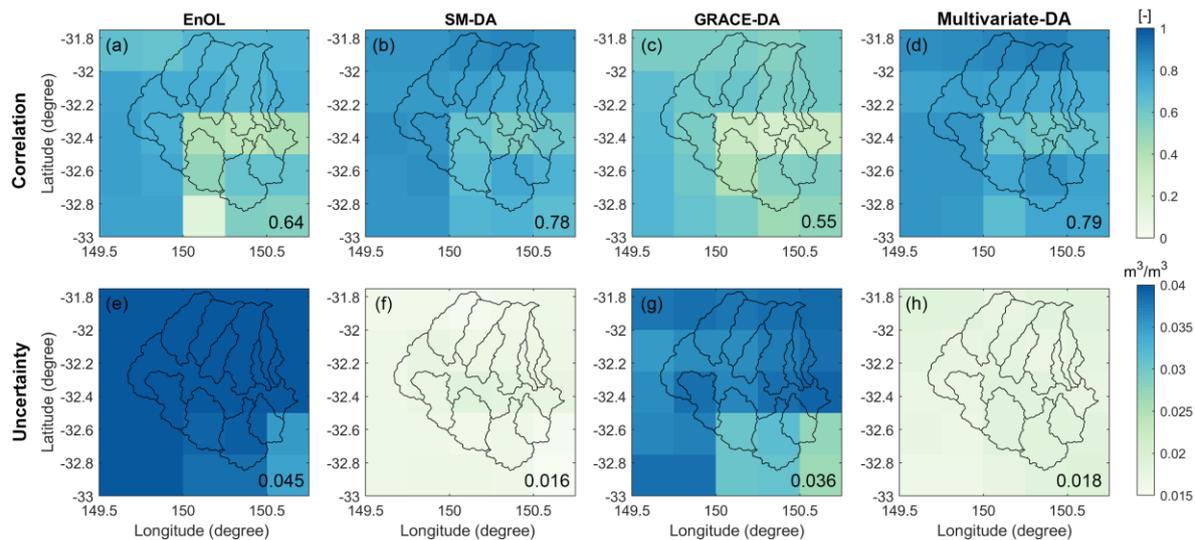
347

348 **4. Results and discussion**

349 **4.1 Impact of DA on soil moisture estimate**

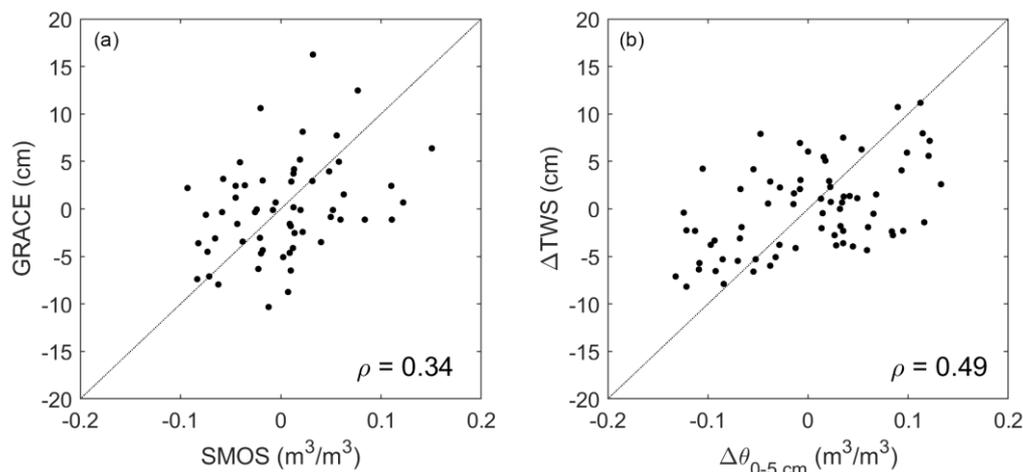
350 The top soil moisture ($\theta_{0-5\text{cm}}$) is estimated from the EnOL and three DA scenarios (SM-only,
351 GRACE-only, and both). The goodness of fit in terms of correlation is evaluated against the SMOS
352 data (Fig. 3, top row) to investigate the impact of different DA scenarios on the $\theta_{0-5\text{cm}}$ estimates.
353 From Fig. 3, the SM DA and the multivariate DA deliver $\sim 0.1 - 0.15$ higher averaged correlation
354 values compared to the EnOL. This is expected, as the SMOS/SMAP data are being integrated into
355 the state estimate (particularly into the $\theta_{0-5\text{cm}}$ component) by the applications of the SM DA and
356 multivariate DA. The Kalman gain attempts to statistically optimize the fit between the $\theta_{0-5\text{cm}}$
357 estimate and the SMOS/SMAP observation, resulting in an improved agreement between them.
358 Similar behavior is also observed from the evaluation with the SMAP data (not shown). Including the
359 SMOS/SMAP data in the assimilation system is proven necessary to improve the $\theta_{0-5\text{cm}}$ estimate.

360 By contrast, GRACE DA reduces the correlation value by ~ 0.1 . The degradation is likely caused by
361 the limited sensitivity of GRACE observations to top soil moisture. The top soil component is
362 strongly governed by high-frequency meteorological forcing (Wu et al., 2002) while GRACE can
363 only observe monthly catchment-averaged TWS changes, which is dominated by the low-frequency
364 variability of deep-water storage components. Also, the degradation of surface SM after assimilating
365 GRACE suggests an inconsistency between the observed and modeled SM-TWS relationship. As
366 shown in Fig 4, the modeled TWS change is less sensitive to the modeled SM change, compared to
367 the corresponding observations. Therefore, correcting the modeled TWS to GRACE may over-correct
368 SM estimates and lead to degraded results. Clearly, assimilating GRACE data alone cannot provide
369 the high spatiotemporal variability essential for modeling the water storage in the top soil layer, and
370 the inclusion of GRACE data tends to have a negative impact on the $\theta_{0-5\text{cm}}$ estimate.



371

372 **Figure 3.** The correlation coefficients (top row) and uncertainty (ensemble spread, bottom row) of the
 373 0 – 5 soil moisture estimates computed between the SMOS data and different DA case studies. The
 374 averaged correlation and error values of the Goulburn catchment are given in each figure.



375

376 **Figure 4.** Scatter plots between the basin-averaged ΔTWS and soil moisture anomaly ((a) GRACE
 377 Vs. SMOS, and (b) CABLE-estimated ΔTWS and $\Delta\theta_{0-5cm}$) of the Goulburn catchment. The
 378 correlation coefficient (ρ) is provided in each figure.

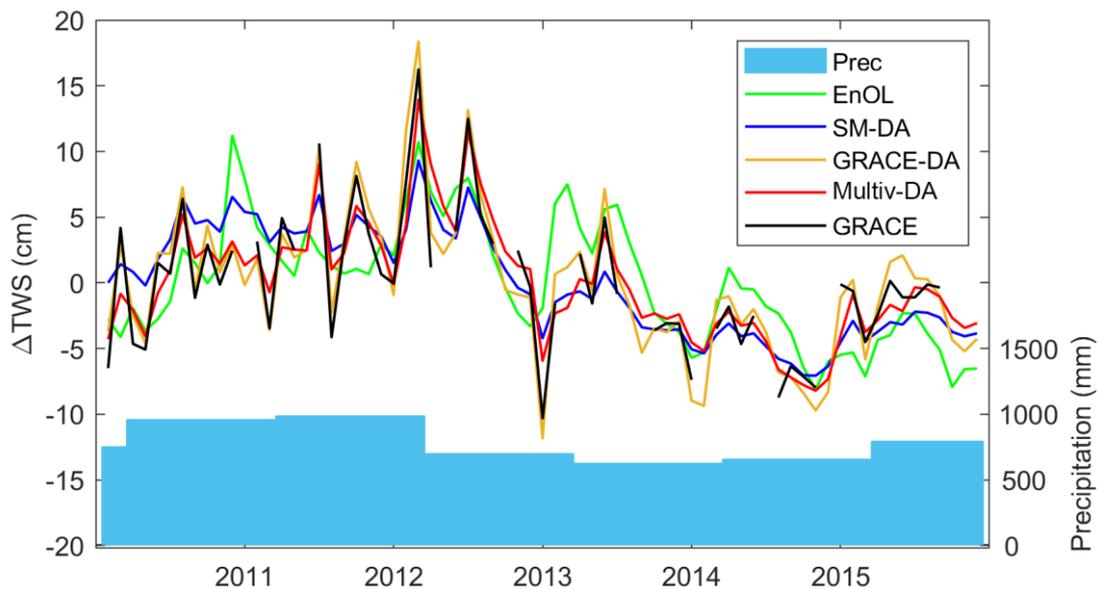
379

380 All DA cases reduce the uncertainty (ensemble spread) of the θ_{0-5cm} estimate (Fig. 3, bottom row).
 381 Compared to the EnOL, the SM DA and multivariate DA reduce the uncertainty by a factor of three
 382 while the GRACE DA reduces the uncertainty by a factor of 1.2. Importantly, the applications of the
 383 SM DA and multivariate DA also lead to an approximately three times lower uncertainty than the
 384 assigned SMOS/SMAP uncertainty value. In addition, it is seen that the uncertainty of the θ_{0-5cm}
 385 estimate is lower in the south-eastern part of the catchment. This is likely influenced by the lower
 386 field capacity associated with lower clay content in the southern region, leading to a small variation of
 387 θ_{0-5cm} and its uncertainty. The spatial pattern of the uncertainty also explains the contribution of
 388 SMOS/SMAP observation. The update is likely limited in the south-eastern part where the model
 389 uncertainty is small. This is apparent in, e.g., Fig. 3b where slightly lower correlation values are
 390 observed mostly in the south-eastern region.

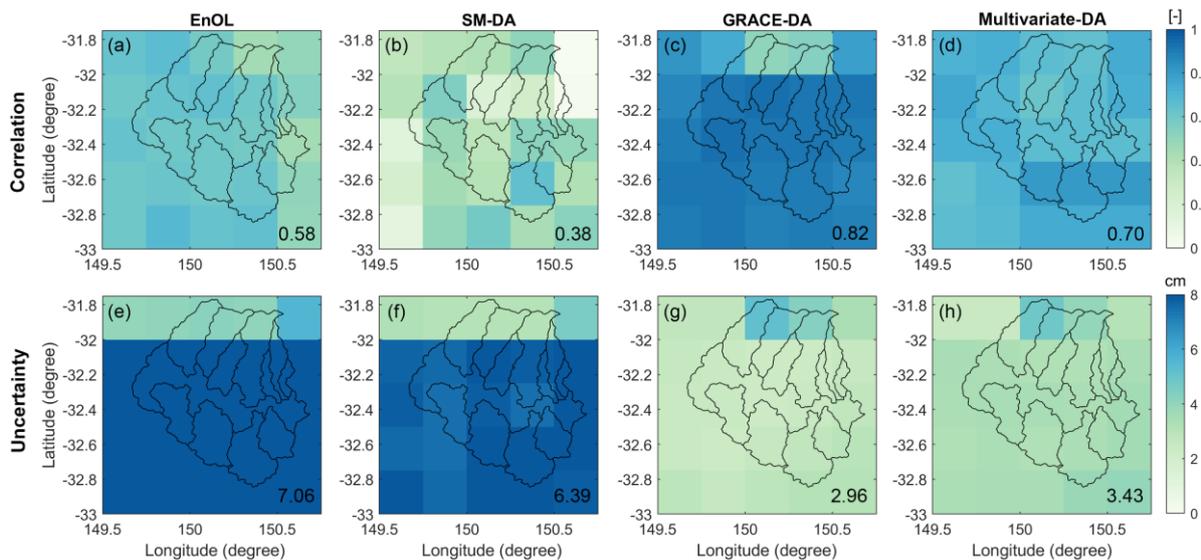
391

392 **4.2 Impact of DA on TWS estimate**

393 The basin-averaged ΔTWS of all three DA cases is shown in Fig. 5. Also, the correlation with respect
 394 to GRACE is shown in Fig. 6 (top row). Assimilating SMOS/SMAP-only yields a negative impact on
 395 the ΔTWS estimates, resulting in a decreased agreement between the state estimate and the GRACE
 396 observation. In the SM DA, the smoother underestimates the annual and inter-annual variability of
 397 ΔTWS and reduces the averaged correlation value by ~ 0.2 (Fig. 6b). The smoothers estimate a set of
 398 the ensemble by optimizing the Kalman gain (or likelihood) function associated only with the θ_{0-5cm}
 399 component while leaving the other storage components unconstrained. Computing the posterior
 400 estimate based on the resulted sample set produces an improved θ_{0-5cm} estimate (see also Sect. 4.1),
 401 but does not necessarily improve the computation of total storage changes. The degradation in ΔTWS
 402 may be due to the fact that the satellite SM observation does not provide information on the total
 403 column water, which is crucial in the accurate distribution of the water through all stores.



404
 405 **Figure 5.** The monthly basin-averaged ΔTWS computed from different DA approaches (SM DA,
 406 GRACE DA, and multivariate DA). The EnOL estimate, the GRACE observation, and the yearly
 407 precipitation accumulated between April and May are also shown for comparison.



408
 12

409 **Figure 6.** The correlation coefficients (top row) and errors (ensemble spread, bottom row) of the
 410 Δ TWS estimate computed between the GRACE observation and different DA case studies. The
 411 averaged correlation and error values of the Goulburn catchment are given in each figure.

412

413 In the GRACE DA, the constraint is applied to the entire water column, leading to an improved
 414 agreement between the Δ TWS estimate and the GRACE observation. The averaged correlation value
 415 is increased by ~ 0.2 (Fig. 6c). The impact of the GRACE DA is clearly seen in the Δ TWS adjustment
 416 before and after March 2012. To evaluate this, the total mass variation in the two periods (January
 417 2010 – March 2012 and April 2012 – December 2015) is computed and shown in Table 2. To
 418 determine the total mass of TWS variation (Gton) in each period, the long-term trend (m/year) is first
 419 estimated, and multiplied by the area of the Goulburn catchment (see Sect. 2.1), the density of water,
 420 and the number of years in that period, respectively. GRACE observes the increased mass estimate of
 421 ~ 0.6 Gton prior to April 2012, which is mainly induced by the 2010 – 2011 La Niña rainfall (see Fig.
 422 5). The EnOL underestimates the mass estimate by ~ 0.1 Gton during this period. The estimate is
 423 improved by the GRACE DA, leading to a $\sim 20\%$ improvement in cross-correlation between the
 424 adjusted mass estimate and GRACE data. Similar behavior is observed during the post La Niña period
 425 (after March 2012) when the GRACE DA produces a $\sim 30\%$ improvement in cross-correlation.
 426 Unlike the GRACE DA, the SM DA cannot improve the mass estimate in both periods due to e.g., the
 427 deficiency of deep-water storage information necessary for the TWS computation.

428

429 **Table 2.** Total mass variations (Gton) estimated from nine different DA case studies, model estimate
 430 (EnOL), and GRACE observation during two periods: January 2010 – March 2012 and April 2012 –
 431 December 2015.

Period	SM DA	GRACE DA	Multivariate DA	EnOL	GRACE observation
Jan 2010 – Mar 2012	0.12	0.64	0.56	0.48	0.61
Apr 2012 – Dec 2015	-0.21	-0.30	-0.34	-0.47	-0.35

432

433 It is apparent that SM DA and GRACE DA are valuable for updating $\theta_{0-5\text{cm}}$ and TWS estimates,
 434 respectively, while they show limited benefit for the estimation of the other components. The
 435 underlying strengths motivate the concept of assimilating the SMOS/SMAP and GRACE observation
 436 simultaneously into the LSM. In the multivariate DA, the $\theta_{0-5\text{cm}}$ and Δ TWS components are adjusted
 437 toward the SMOS/SMAP and GRACE observation, respectively, resulting in the final state estimates
 438 that agree with both observations. The Δ TWS estimated with multivariate DA agrees better with the
 439 GRACE observations by ~ 0.12 in cross-correlation (Fig. 6d) and, simultaneously, the $\theta_{0-5\text{cm}}$ estimate
 440 presenting better correlation by > 0.1 with SMOS/SMAP data (see Fig. 3b). Consequently, the
 441 multivariate DA improves the mass estimate during the La Niña period (Table 2).

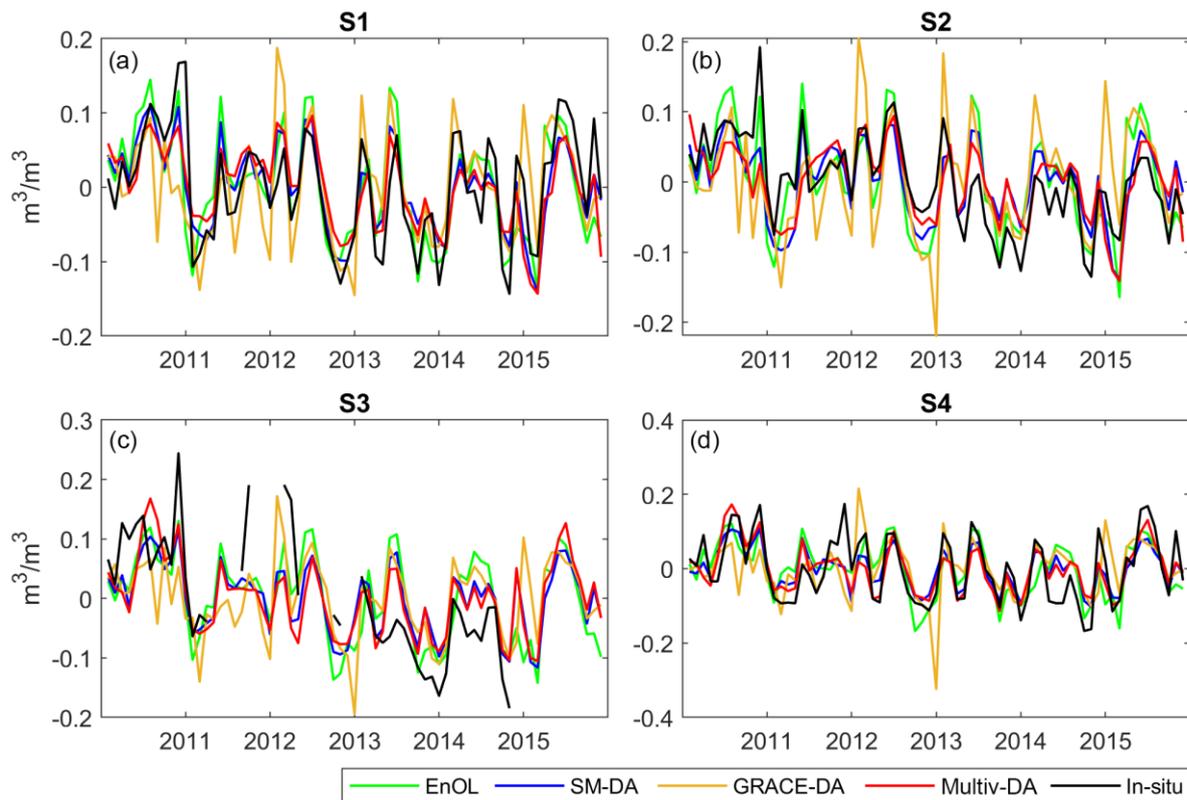
442 The GRACE DA and multivariate DA reduce the TWS uncertainty by more than a factor of 2 (Fig. 6,
 443 bottom row). As expected, the SM DA cannot deliver a reliable TWS estimate, as seen in the
 444 uncertainty which is approximately twice that obtained from the GRACE DA and multivariate DA.

445

446 **4.3 Validation with in situ data**

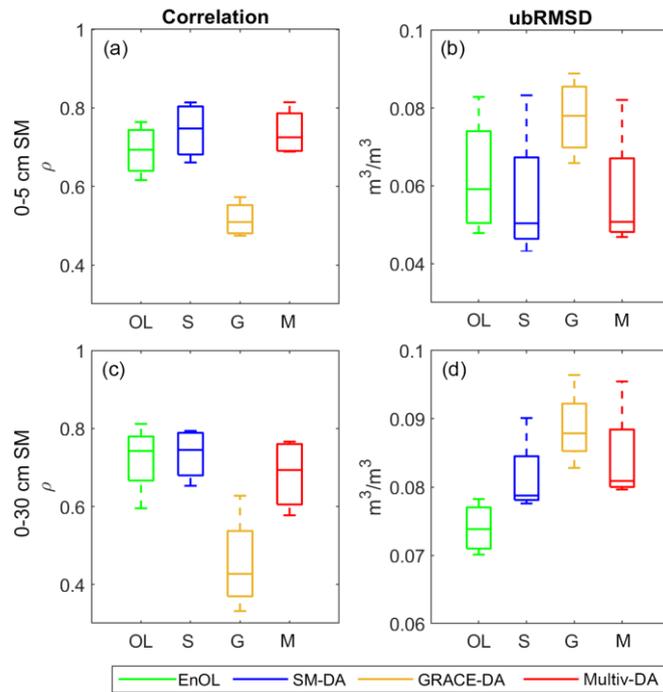
447 **4.3.1 Soil moisture**

448 The $\theta_{0-5\text{cm}}$ variations estimated from all DA case studies are validated against the in-situ data at S1 –
 449 S4 (Fig. 7). The validation is conducted in terms of correlation and ubRMSD, and the estimated
 450 values are shown in Fig. 8. CABLE performs remarkably well in the estimation of $\theta_{0-5\text{cm}}$, and
 451 provides a good agreement with the in situ data at all locations with an averaged correlation value of
 452 ~ 0.69 (see EnOL in Fig. 8a). The SM DA and multivariate DA increase the correlation value further
 453 by $\sim 7\%$ (from ~ 0.69 to ~ 0.73) and decrease the ubRMSD by $\sim 11\%$. The improved result is
 454 anticipated since the satellite SM observation is used in the SM DA and multivariate DA. By contrast,
 455 the GRACE DA shows an apparent negative impact on the $\theta_{0-5\text{cm}}$ estimate (see, Fig. 8a, b).
 456 Comparing to the EnOL, the GRACE DA overestimates $\theta_{0-5\text{cm}}$ by a factor of 1.5 (ubRMSD), and
 457 decreases the correlation by 50%. Poor performance is due to the insensitivity of GRACE data to the
 458 signal associated with the top soil component as described in Sect. 4.1 and 4.2.



459

460 **Figure 7.** The monthly “0 – 5 cm” soil moisture variations estimated at S1 – S4 pixels computed from
 461 different DA approaches (SM DA, GRACE DA, and multivariate DA). The EnOL estimates and the
 462 in situ soil moisture data are also shown for comparison.



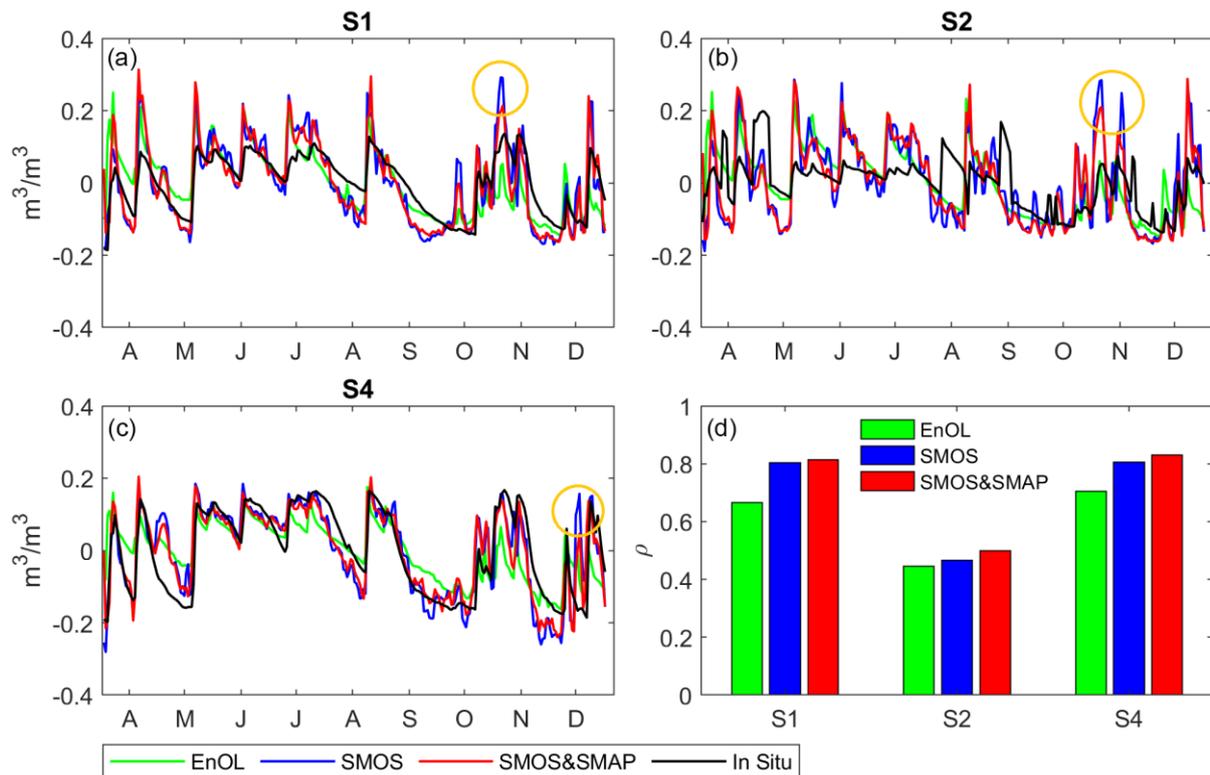
463

464 **Figure 8.** The correlation coefficients (a, c) and unbiased root mean square differences (ubRMSD; b,
 465 d) of the 0 – 5 cm soil moisture (top row) and 0 – 30 cm soil moisture (bottom row) computed from
 466 the estimate of different DA case studies at S1 – S4 (S: SM DA, G: GRACE DA, M: Multivariate
 467 DA). The statistical results of the EnOL (OL) are also shown.

468 The $\theta_{0-30\text{cm}}$ variation is also validated against the in-situ data with the statistical results shown in
 469 Fig. 8 (bottom row). CABLE provides a very accurate $\theta_{0-30\text{cm}}$ component with a correlation value of
 470 almost 0.7 (Fig. 8c). Unlike the $\theta_{0-5\text{cm}}$, the SM DA and multivariate DA do not improve the
 471 correlation and ubRMSD values of the $\theta_{0-30\text{cm}}$ estimate. This is consistent previous studies that
 472 found that the benefit of surface SM DA in root zone SM estimates depends on the accuracy of model
 473 physics (Dunne et al., 2007; Kumar et al, 2009). In line with the analysis found in Fig.4, GRACE DA
 474 also reduces the quality of the $\theta_{0-30\text{cm}}$ estimate, seen from both metrics.

475 The benefit of including the SMAP data in the DA system is evaluated. The multivariate DA results
 476 from two case studies using SMAP data between March and December 2015 are compared with the
 477 in-situ data at S1, S2, and S4 (Fig. 9a – c). The in-situ data at S3 are not available during this
 478 validation period. In all locations, the daily $\theta_{0-5\text{cm}}$ estimates of the SMOS-only assimilation and the
 479 SMOS/SMAP assimilation are very similar and visibly show a better agreement with the in-situ data
 480 (comparing to the EnOL). The correlation value is increased to almost 0.2 (e.g., at S1, Fig. 9d), and
 481 the highest correlation value is seen when the SMAP data is included in the DA system (~3 % higher
 482 compared to the SMOS-only assimilation). The application of the SMOS/SMAP assimilation also
 483 reduces the spurious peaks of the $\theta_{0-5\text{cm}}$ estimate, e.g., in October 2015 (Fig. 9a, b) and November
 484 2015 (Fig. 9c), leading to a better agreement with the in-situ data. Evidently, the SMAP data should
 485 be considered in the DA process to maintain the accuracy (in terms of agreement with the in situ data)
 486 of the $\theta_{0-5\text{cm}}$ estimate in the Goulburn catchment.

487

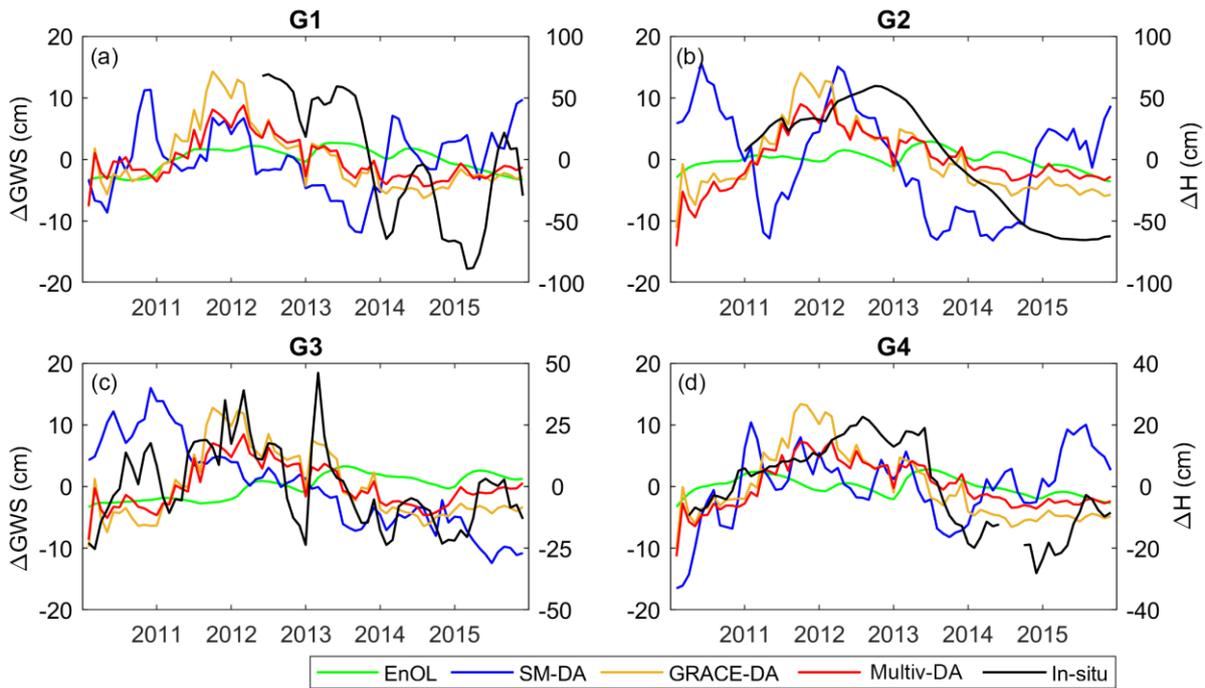


488

489 **Figure 9.** The daily 0 – 5 soil moisture variations estimated at S1 (a), S2 (b), and S4 (c) pixels from
 490 the EnOL estimate, the SMOS-only DA estimate, the SMOS/SMAP DA estimate, and the in situ data
 491 between March and December 2015. Circles indicate the spurious peaks found in SMOS-only DA
 492 estimate. The correlation coefficients between the in situ data and the results of the EnOL, the SMAP-
 493 only DA, and the SMOS/SMAP DA are shown in (d).

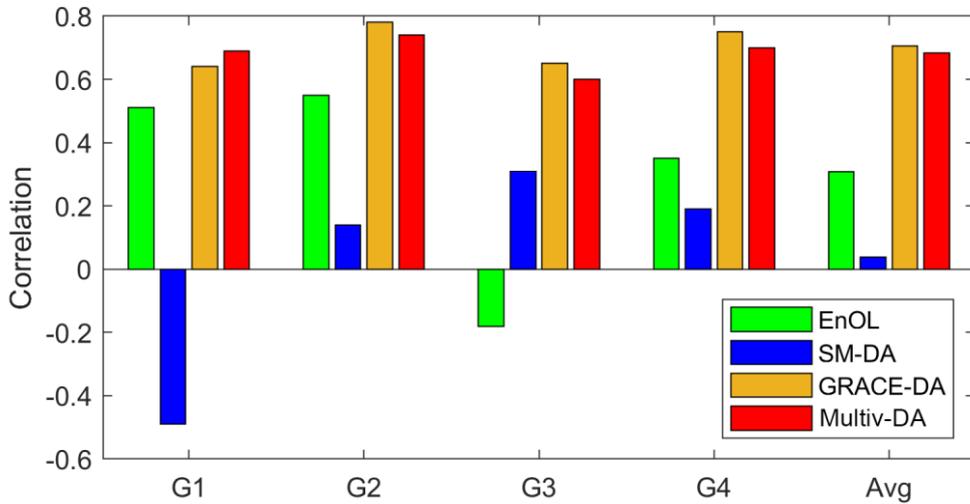
494 **4.3.2 Groundwater storage**

495 The Δ GWS estimates are compared with the in-situ groundwater level anomalies (Δ H) at G1 – G4
 496 (Fig. 10), and the averaged correlation coefficients are shown in Fig. 11. In Fig. 10, the application of
 497 the SM DA leads to an incorrect groundwater storage estimate with a large disagreement between the
 498 Δ GWS estimate and Δ H, particularly at G1 where the correlation value is as low as -0.6. The poor
 499 performance can be attributed to the lack of groundwater information in the satellite SM observation
 500 (see Sect. 4.1 and 4.2). The Δ H shows a very similar temporal variation in all G1 – G4 locations. The
 501 different scale between Δ GWS and Δ H likely causes the visual phase shift seen in Fig. 10. Applying a
 502 specific yield (e.g., ranging between 0 and 1) to Δ H could reduce the magnitude of the right axis, and
 503 led to the reduction of visual phase shift. However, the conversion is not performed due to the absence
 504 of specific yield as described in Sect. 2.5. The temporal variations of Δ H follow those of the Δ TWS
 505 estimate and the GRACE observations (see Fig. 5). Δ H (and Δ TWS) increases under the influence of
 506 the La Niña rainfall in 2011 – 2012 and decreases afterward. The similarity suggests that GRACE is
 507 sensitive to the signal of the groundwater store more than the shallow storage component. In
 508 particular, the groundwater level data (Δ H) are correlated throughout the catchment with the cross-
 509 correlation of ~0.9 (see Fig. 6 in Tangdamrongsub et al. (2017a)). The assimilation of GRACE data
 510 (in both GRACE DA and multivariate DA) increases the correlation between the Δ GWS estimate and
 511 Δ H changes in each grid by a factor of 2, compared to the EnOL estimate.



512

513 **Figure 10.** The monthly groundwater storage variations (ΔGWS) at G1 – G4 pixels computed from
 514 different DA approaches (SM DA, GRACE DA, and multivariate DA). The EnOL estimates and the
 515 in situ groundwater level variations (ΔH) are also shown for comparison.



516

517 **Figure 11.** The correlation coefficients of the ΔGWS estimates at (a) G1, (b) G2, (c) G3, and (d) G4
 518 pixels computed from EnOL and different DA case studies. The averaged correlation values (Avg) of
 519 G1 – G4 are also shown.

520

521 The EnOL-simulated ΔGWS shows smaller variations compared to the DA estimate and ΔH . CABLE
 522 models the unconfined aquifer using a simple groundwater model (Decker, 2015; Decker and Zeng,
 523 2009; Niu et al., 2007; Vergnes et al., 2012) that calculates the groundwater recharge based on the
 524 available water after vertical redistribution between the soil layers. This simplification might lead to
 525 an enclosed groundwater component in the deep soil layer when the distributing water does not reach
 526 the defined field capacity. In such a case, groundwater recharge is not accounted for correctly, and the
 527 groundwater storage changes become small. The soil and groundwater components are not efficiently
 528 separated, and the variation of the ΔGWS estimate is likely presented in the deep soil layer.

529 Assimilating GRACE-only always shows a better performance in the Δ GWS estimate and provides
530 ~29 % higher average correlation compared to assimilating both GRACE and SMOS/SMAP
531 measurements. In the multivariate DA, Δ GWS is updated by the GRACE DA (step 2 in Fig. 2c) after
532 the application of the SM DA (step 1 in Fig. 2c). The application of the SM DA (in the multivariate
533 DA) likely decreases the uncertainty of the state estimate, which consequently reduces the
534 contribution of GRACE in the analysis step of the GRACE DA. Rescaling the GRACE uncertainty
535 could increase the contribution of the GRACE observation (e.g., Tian et al., 2017).

536

537 **5. Conclusions**

538 This study evaluates three different DA schemes to assimilate different combinations of satellite
539 observations (SMOS/SMAP, GRACE, and both (SMOS/SMAP and GRACE)) in the Goulburn
540 catchment, Australia. Validation against the in-situ data reveals that the performance of the DA in
541 estimating soil moisture and groundwater storage highly depends on the choice of the observation
542 type. The application of the SM DA significantly improves the top (0 – 5 cm) soil moisture but
543 degrades the groundwater component, whereas the GRACE DA improves only the Δ GWS estimate.
544 Applying the multivariate DA simultaneously increases the accuracy of the soil moisture and
545 groundwater storage estimates, though at a slightly lesser degree of improvement compared to the
546 single observation DA case.

547 The application of the SM DA underlines the importance of the SMOS/SMAP data on the SM
548 estimate, by increasing the 0 – 5 cm correlation with in situ observations by up to 7 %. The benefit on
549 the 0 – 30 cm soil moisture and groundwater component is minor or negative, which is in line with
550 several previous studies. For example, Blankenship et al. (2016), Kolassa et al. (2017), Ridler et al.
551 (2014) and Tian et al. (2017), who reported a detrimental impact on the root zone and deep storage
552 components. SM DA significantly reduces the uncertainty of storage in the top 0 – 5 cm soil layer but
553 does not have an impact on the TWS uncertainty. The constraint solely in the top soil moisture
554 component by the SM DA does not necessarily have a positive effect on the entire water column. We
555 also found that assimilating both SMOS and SMAP data simultaneously is recommended in the
556 Goulburn catchment. The advantage of multivariate SM DA is also found in Lievens et al. (2017),
557 Kumar et al. (2018), Jasinski et al. (2019). However, it should be noted that SMOS and SMAP soil
558 moisture may have potentially common systematic errors, which may affect the observation error
559 matrix. Future studies should explore the magnitude of SMOS-SMAP error cross-correlation and its
560 impact on the DA results.

561 The GRACE DA demonstrates an outstanding example of improving the groundwater storage of the
562 Goulburn catchment, particularly at a finer spatial resolution (~25 km) compared to GRACE's
563 intrinsic resolution (>100 km). As the groundwater variation of the Goulburn catchment is likely to be
564 spatially correlated due to the large unconfined aquifer (Tangdamrongsub et al., 2017a), assimilating a
565 coarser spatial scale Δ TWS from the GRACE observation can benefit the groundwater estimate even
566 in the smaller individual grid cell. GRACE DA leads to the improved groundwater estimate by
567 increasing the correlation to independent in situ groundwater level data. However, assimilating
568 GRACE into LSM does not provide a positive impact on the top or surface SM components. This is
569 consistent with the conclusions of Li et al. (2012) and Tian et al. (2017). GRACE DA significantly
570 reduces the uncertainty of the TWS estimate but has only a minor impact on the SM uncertainty. It is
571 known that GRACE is sensitive to the signal of the entire water column, dominated by the processes
572 in deeper layers. The GRACE DA might therefore adversely distribute the deep water storage signals
573 into the shallow one.

574 Multivariate DA provides an improvement over both SM and Δ GWS estimates. Assimilating the
575 satellite soil moisture and GRACE data together allows the high-frequency components to be adjusted

576 by the SM DA while the low-frequency signal is corrected by the GRACE DA, leading to the
577 increased correlation values of both the 0 – 5 cm soil moisture (by ~7 %) and Δ GWS estimates (by
578 ~65 %), compared to the independent in situ data. However, the multivariate DA does not outperform
579 the SM DA or the GRACE DA in the separate estimation of the “0 – 5 cm” soil moisture and Δ GWS.
580 The DA approach optimized the model states with multiple cost functions relevant to shallow and
581 deep groundwater storage changes (e.g., minimizing the residuals against both SMOS/SMAP and
582 GRACE), resulting in an optimal solution that is not closer to one particular observation, as also
583 found by Tian et al. (2017).

584 With the increased availability of satellite retrievals and ground measurement networks, multivariate
585 DA can be an effective tool to exploit diverse observations. The multivariate DA presented in this
586 study can be extended to include different types of new observations (e.g., soil moisture from
587 Sentinel-1 (Lievens et al., 2017), Δ TWS from GRACE Follow-On (Flechtner et al., 2014), snow
588 water equivalent from SnowEx (Kim, 2017)) with simple modification of the measurement operator
589 as described in Sect. 3.2. Ongoing research is focused on the sensitivity to the selected window
590 length (L) of the smoother (Dong et al., 2015) and applications over regions with different climate
591 conditions (e.g., snow-covered basins).

592

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600 information provided in Section 2.

601

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