
Covariance Analysis and Sensitivity Studies for GRACE Assimilation into WGHM

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Abstract

An ensemble Kalman filter approach for improving the WaterGAP Global Hydrology Model (WGHM) has been developed, which assimilates Gravity Recovery And Climate Experiment (GRACE) data and calibrates the model parameters, simultaneously. The method uses the model-derived states and satellite measurements and their error information to determine updated water storage states. However, due to the fact that hydrological models do not provide any error information, an empirical covariance matrix needs to be calculated. In this paper, therefore, we analyse the combined state and parameter covariance matrix of WGHM. We found that high correlations of up to 0.75 exist between calibration parameters and storage compartments, and that these allow for an efficient calibration. In addition, a sensitivity analysis is performed to identify those parameters that the water compartments are most sensitive to. The performed analysis is important, since GRACE cannot observe the model parameters directly. We found that those parameters, which the water storage is most sensitive to, differ not only regionally, but also with respect to the water compartments. Not unexpected, some climate input multipliers implemented in our model version have an overall strong influence. We also found that the degree of sensitivity changes temporally, e.g. between 0 (in summer) and 0.5 (in winter) for the snow storage.

Keywords

Assimilation • Calibration • GRACE • Sensitivity • WGHM

1 Introduction

The global water cycle is one of the most important processes that ensure life on Earth. Modelling of continental hydrology contributes to its understanding and quantification. A global representation of the terrestrial water cycle is, e.g. provided by the WaterGAP Global Hydrology Model

(WGHM), which models the vertical and horizontal water fluxes on a 0.5° grid over the land area. A detailed description of the model can be found e.g. in Döll et al. (2003) and Müller Schmied et al. (2014). However, the degree of a successful representation of the reality is limited due to the simplified representation of hydrological processes and due to the uncertainties of input data, e.g. empirical model parameters, climate forcing and water use data. On the other hand, the Gravity Recovery And Climate Experiment (GRACE) satellite mission (Tapley et al. 2004) observes the Earth's time variable gravity field and methods have been developed that allow one to separate the column-integrated sum of the terrestrial water storage from the total mass signal. Therefore, these measurements can be used to improve hydrological models by calibrating their parameters or adjusting their states to the observations.

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Two main approaches exist so far for the improvement of a hydrological model by using GRACE measurements. Werth and Günthner (2009) used filtered basin means of GRACE total water storage (TWS) changes to improve WGHM. Their aim was the calibration of the model parameters. Zaitchik et al. (2008) used the same kind of observations to improve NASA's catchment land surface model (CLSM) by assimilating GRACE data into it. To this end, they used an ensemble Kalman smoother method.

An ensemble Kalman filter (EnKF) that simultaneously calibrates the parameters of WGHM and assimilates GRACE data into it has been proposed in Schumacher (2012). In contrast to the previous studies, the approach presented here uses TWS changes from GRACE defined on a grid for the calibration and assimilation. Furthermore, the full spatio-temporal GRACE TWS changes error information was considered in the method. For implementing a Kalman filter approach, an empirical model covariance matrix of WGHM has to be determined. This is due to the fact that hydrological models do not provide error information by default. A detailed description of the method is given by Eicker et al. (2014) in which investigations on the Kalman filter gain matrix are presented.

In this paper, we focus on the analysis of the combined model parameter-state covariance matrix to identify those parameters that the water compartments are most sensitive to. The results are presented with respect to the Mississippi River Basin. In addition, a detailed sensitivity analysis was performed with the aim (a) to assess the results of the local model covariance matrix and (b) to identify those parameters with the highest model sensitivity for the 33 largest river basins in the world. These results are compared to those in Werth and Günthner (2009). Additionally, we carried out investigations on the water compartments and on the evolution of sensitivity over time.

2 Data

2.1 WGHM

Within the EnKF approach, the modeled water storages of canopy, snow, soil, river, surface water bodies and groundwater from the current WaterGAP version 2.2 (Müller Schmied et al. 2014) are integrated with the observed TWS changes from GRACE. To determine improved water storage values, the error information of model and measurements are weighted against each other (Schumacher 2012). Since WGHM does not provide error information, an empirical model covariance matrix has to be determined. Here, the influence of the empirical model input parameters on the modeled water storages is considered. Some of these parameters describe physio-geographic characteristics, e.g.

Table 1 Calibration parameters of WGHM with identification number (IN) and original value

IN	Calibration parameter	Value
1*	Root depth multiplier	1
2*	River roughness coefficient multiplier	1
3	Lake depth	5 m
4	Wetland depth	2 m
5	Surface water outflow coefficient	0.01/day
6*	Net radiation multiplier	1
7	Priestley-Taylor coefficient (humid)	1.26
8	Priestley-Taylor coefficient (arid)	1.74
9	Max. daily potential evapotranspiration	15 mm/day
10	Max. canopy water height per leaf area	0.3 mm
11*	Specific leaf area multiplier	1
12	Snow freeze temperature	0°C
13	Snow melt temperature	0°C
14*	Degree day factor multiplier	1
15	Temperature gradient	0.006°C/m
16*	Groundwater factor multiplier	1
17*	Max. groundwater recharge multiplier	1
18	Critical precipitation for groundwater recharge	10 mm/day
19	Groundwater outflow coefficient	0.01/day
20*	Net abstraction surface water multiplier	1
21*	Net abstraction groundwater multiplier	1
22*	Precipitation multiplier	1

Parameters, marked with (*), are not integrated in the original WaterGAP 2.2 version, but are extra parameters within the adapted version used here

the lake depth. Other parameters are conceptual, such as the groundwater outflow coefficient. Whereas it is common that only one parameter associated with the soil compartment (runoff coefficient γ) is used for calibration to fit mean annual discharge to observed one (Döll et al. 2003), Werth and Günthner (2009) used the six to eight most sensitive ones per river basin. Those calibration parameters, which are considered in our EnKF approach, are listed in Table 1.

2.2 GRACE TWS Changes

For the calibration and assimilation approach the ITG-GRACE2010 monthly GRACE solutions were used for which the full error information is available (<http://www.igg.uni-bonn.de/apmg/index.php?id=itg-grace2010>). $0.5^\circ \times 0.5^\circ$ TWS grids are derived following Wahr et al. (1998). The full monthly covariances of potential coefficients were propagated to TWS. A suitable filter technique and an approach to account for leakage effects due to filtering are under investigations and will be reported in future work. However, these choices do not affect the results presented here.

3 Method

3.1 Empirical Model Covariance Matrix

To estimate a combined empirical covariance matrix of the states and parameters, first of all, a priori probability density functions (PDF) have been chosen based on literature (Kaspar 2004) and our own experience of more than 10 years of model development for the model parameters. One of the parameters was assumed to be uniformly distributed, the others were assumed to have a triangular distribution, which can be symmetric or asymmetric. An ensemble of $N = 60$ calibration parameter sets was generated by using a Monte Carlo approach taking into consideration the above mentioned PDFs. For each ensemble member, the model was run globally from 2002 to 2009 for which ITG-GRACE2010 solutions are also available. Identical start values of the cell water storage compartments were used for each run. Time series of monthly averaged water storage states corresponding to each grid cell were obtained as model output for each ensemble member. The monthly regional empirical covariance matrix \mathbf{C}_e for one specific river basin was calculated by using the parameter \mathbf{p} and model state \mathbf{s} ensembles (e.g., Evensen 2009)

$$\mathbf{C}_e = \frac{1}{N-1} \mathbf{X}'(\mathbf{X}')^T. \quad (1)$$

The mean reduced model prediction matrix \mathbf{X}' contains the storage in all compartments for each grid cell in the specific basin and the calibration parameter values for each of the ensemble members in its columns. The covariance matrix consists of three blocks

$$\mathbf{C}_e = \begin{bmatrix} \mathbf{C}_e(\mathbf{s}^-, \mathbf{s}^-) & \mathbf{C}_e(\mathbf{s}^-, \mathbf{p}^-) \\ \mathbf{C}_e(\mathbf{p}^-, \mathbf{s}^-) & \mathbf{C}_e(\mathbf{p}^-, \mathbf{p}^-) \end{bmatrix}. \quad (2)$$

The first block $\mathbf{C}_e(\mathbf{s}^-, \mathbf{s}^-)$ contains the error information with respect to the predicted model states, the second block $\mathbf{C}_e(\mathbf{p}^-, \mathbf{p}^-)$ is related to the parameters. The last block $\mathbf{C}_e(\mathbf{s}^-, \mathbf{p}^-)$ contains the relation between the model states and parameters. To determine those parameters, which the model compartments are most sensitive to, the correlations between each parameter and the basin averaged water compartments were calculated. Since GRACE does not observe the parameters directly, the correlations justify whether the observations will contribute in calibrating the model parameters.

3.2 Sensitivity Analysis

Another possibility to identify those conceptual parameters that relate to large model sensitivities can be derived

by performing a sensitivity analysis (e.g., Hamby 1994). Here, the sensitivity index (SI), which is a simple approach, and the Spearman's rank correlation coefficient (SRCC), which was used in Güntner et al. (2007), are chosen as a measure of sensitivity. To determine the SI, first realisations of a single model parameter are generated while considering the others as constant. The SI measures the influence of one single input parameter on the model output. Therefore, the interpretation of the SI is straight forward: It corresponds to a model covariance matrix for which only one calibration parameter set is introduced while the others are constant (not shown here). Note that in contrast, ensembles of all model parameters were generated simultaneously when using the SRCC for assessment of sensitivity. Here, the correlations of the model parameters are considered. This corresponds to the information in the empirical model covariance matrix, which is calculated after running the model with an ensemble of all input parameters (Sect. 1).

3.2.1 Sensitivity Index

The SI is a measure that reflects the relative difference between the minimum and maximum model outputs S_{\min} and S_{\max} when generating an ensemble of one model input parameter with the others being constant (Hoffman and Gardner 1983). SI is calculated by scaling the difference between the minimum and maximum water storage output within the ensemble as

$$SI = \frac{S_{\max} - S_{\min}}{S_{\max}}. \quad (3)$$

Although SI is a simple approach to identify parameters, which the water compartments are most sensitive to, its disadvantage is that it does not take the correlations between parameters into account.

3.2.2 Spearman's Rank Correlation Coefficient

Unlike SI, the SRCC also considers the correlations between the calibration parameters. Further, it allows one to account for nonlinear model equations by performing a rank transformation of the parameters and states (Iman and Conover 1979). To apply this approach, sets of all parameters were generated by using their given PDFs simultaneously. The calibration parameter values and model output are sorted in ascending order by their values leading to their ranks. Finally, the Pearson's correlation coefficient is determined with the exception that the ranks of the i -th parameter R_{P_i} and the water states R_S are used instead of their values (Hamby 1994)

$$\rho_i = \frac{\sum_{n=1}^N (R_{P_{in}} - \overline{R_{P_i}})(R_{S_n} - \overline{R_S})}{\sqrt{\sum_{n=1}^N (R_{P_{in}} - \overline{R_{P_i}})^2 \sum_{n=1}^N (R_{S_n} - \overline{R_S})^2}}. \quad (4)$$

The results of the sensitivity analyses can be used to verify the parameter-state correlations, which are empirically determined as entries of the model covariance matrix.

4 Results and Discussion

The analysis of the model covariance matrix and the sensitivity analysis has been performed for all water compartments in the Mississippi River Basin. The results are shown for the snow and soil compartment to provide an example.

4.1 Correlations Between Model States and Parameters

The correlations between the 22 calibration parameters and the snow water storage for each grid cell in the Mississippi River Basin were determined for the winter (Fig. 1a) and the summer season (Fig. 1b). During winter, a high positive correlation was identified with two of the parameters and in most of the cells. Negative correlations were identified between a few parameters and some of the cells. During summer, nearly no correlations were found, since there is usually no snow in the Mississippi Basin. To identify those parameters, which the water compartments are most sensitive to, the empirical covariance matrices were calculated for each month of 2008 considered as the start of the integration of GRACE data. Then a basin mean of the water compart-

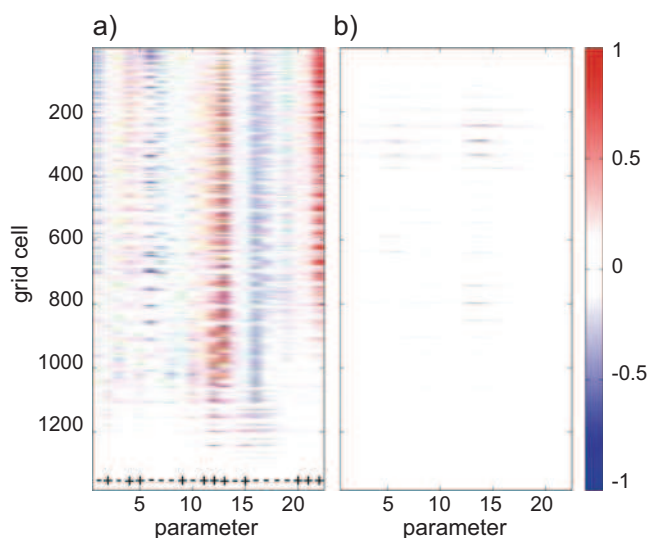


Fig. 1 Correlations between the 22 model parameters and the snow storage in each cell of the Mississippi River Basin for the (a) winter and (b) summer season. See Table 1 for parameter names. In (a) the *plus* and *minus* signs indicate whether the correlation is positive or negative

ments was determined. The time evolution of the correlations between the parameters and the averaged snow and soil compartment are shown in Fig. 2. Between the snow compartment and the snow melt temperature, precipitation multiplier, and groundwater factor multiplier, high correlations exist during winter (Fig. 2a). The precipitation multiplier represents a calibration factor applied to the observed daily precipitation values. Scaled precipitation, which was stored as snow, melts when the actual temperature is higher than the snow melt temperature. The groundwater factor multiplier represents a scaling factor for the calculated groundwater recharge. Between the soil compartment and the root depth multiplier, a calibration factor for the average root depth of plants, and two parameters to determine the potential evapotranspiration, high correlations were found all over the year (Fig. 2b). In the original model version all multipliers are one, i.e. the factors are now introduced for model calibration. Note that regarding Fig. 2a, one observes almost no ensemble spread over the months 4–10, since there is usually no snow in the Basin (see Fig. 1b). This means that these parameters can only be updated during winter. In contrast, the parameters with respect to the soil compartment can be calibrated during all seasons. This indicates nicely that the influence of GRACE differs in each month, since the degree of sensitivity changes over time. In addition, these results suggest that the parameters have to be calibrated at least for a full year, since the determination of e.g., an updated snow melt or freeze temperature during summer is not possible.

4.2 Regional Sensitivity Analysis

By using the SI, the high correlation between the snow storage and the snow melt temperature, and precipitation multiplier respectively was confirmed (Fig. 2c). We found, however, that the groundwater factor multiplier has no impact on the snow storage when measured by the SI. The magnitude of the correlations, when evaluating the model covariance matrix or the SI, is different: e.g. the maximum correlation value concerning the snow melt temperature is 0.5 (Fig. 2a) or 0.8 (Fig. 2c) respectively. This is mainly due to the fact that in case of the first method sets of all parameters were generated, while only a set of one parameter is generated in case of the SI. However, the interpretation of both approaches is the same: The snow melt temperature is the most important parameter with respect to the snow compartment. In summer, it is not possible to update parameters that are directly associated with the snow storage, since no correlations exist. For the soil compartment, the parameters, which were identified by analysing the covariance matrix, were also confirmed by evaluating the SI (Fig. 2d).

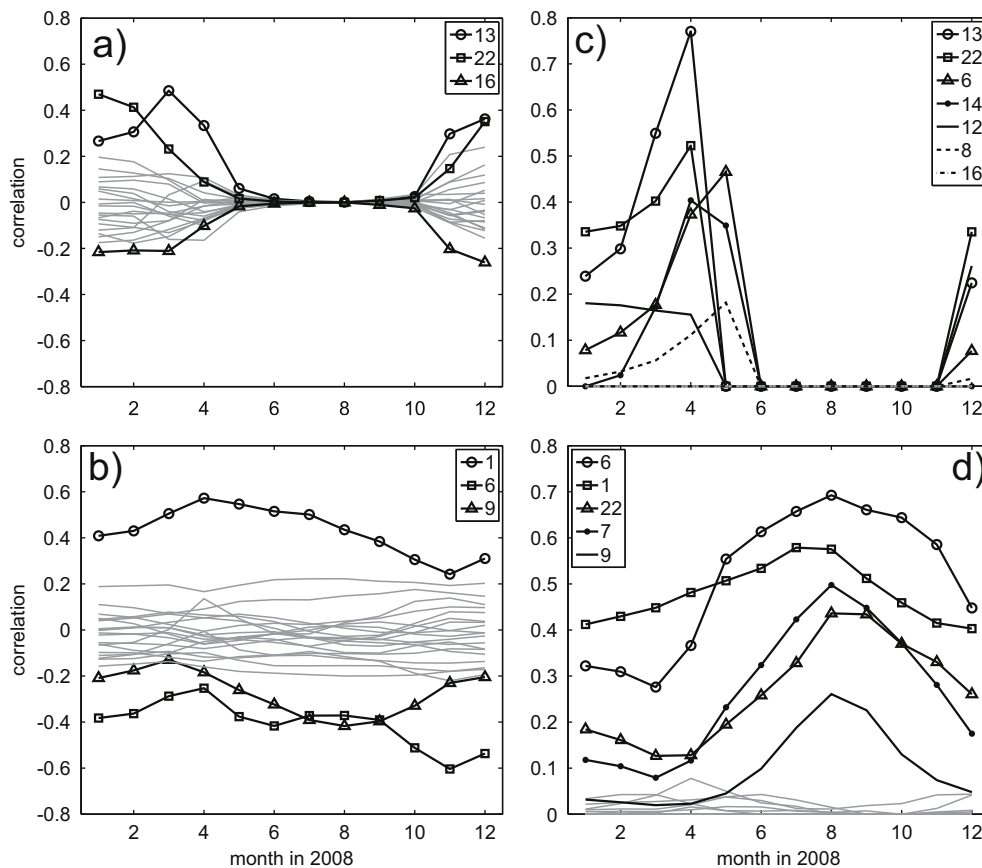


Fig. 2 Time evolution of the correlations between the 22 model parameters and the basin mean of the (a, c) snow and (b, d) soil compartment evaluating the empirical model covariance matrix (a, b) and using the sensitivity index (c, d). The parameters, which have the highest

correlations regarding the averaged compartment states, are listed in the legend. The *gray lines* belong to the other parameters. See Table 1 for parameter names

Considering the SRCC, all parameters with high correlations for the snow and soil compartment were confirmed (not shown here). This includes even the groundwater factor multiplier for the snow. It appears this correlation is introduced through joint dependence on the other perturbed parameters, and thus invisible for the SI.

In the developed EnKF approach, the empirical model covariance matrix, which is computed by first generating an ensemble of all model input parameters, is used in order to determine the updated model states and calibration parameters. This allows the consideration of the parameter, state, and parameter-state correlations in the assimilation and calibration procedure.

4.3 Global Sensitivity Analysis

In addition to the regional analysis, we also performed a global sensitivity analysis to identify the parameters with the highest model sensitivity for the 33 largest river basins in the

world. Here, the SRCC was calculated between the calibration parameters and the mean TWS. Different parameters, which the modeled TWS output is most sensitive to, were found for the basins (Figs. 3 and 4). For example, the TWS in the Mississippi River Basin reacts the most sensitive to the net radiation multiplier, as in numerous of the basins. It seems that this calibration parameter has, along with the river roughness coefficient and precipitation multiplier, an overall strong influence. To make the results comparable to the studies of Güntner et al. (2007) and Werth and Günthner (2009), the SRCC was also determined between the calibration parameters and the mean annual amplitude of TWS as a measure for sensitivity (not shown here). Our results confirm some of those parameters with large model sensitivity in the world's largest river basins that were found in these studies, e.g. the root depth multiplier and snow melt temperature regarding the Mississippi River Basin. In contrast to these studies, in which neither a net radiation nor a precipitation multiplier were introduced, a strong dependence of the TWS on the climate input was found here.

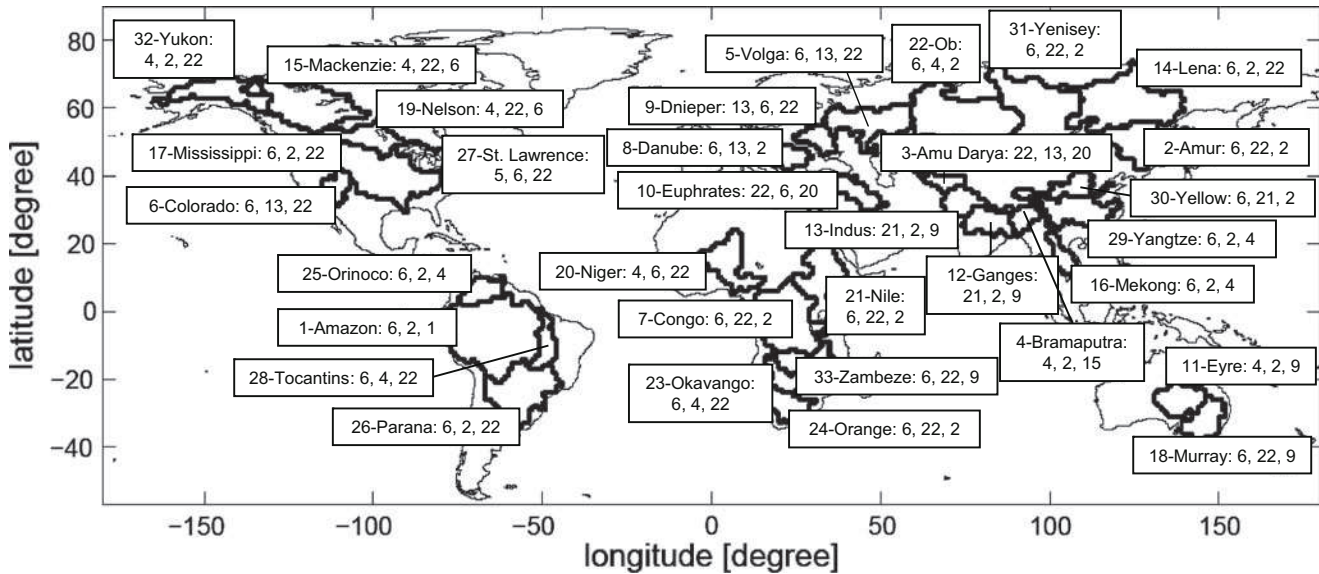


Fig. 3 The three parameters, which the monthly mean TWS output of WGHM is most sensitive to, in the 33 largest river basins of the world. See Table 1 for parameter names. The in the adapted model

version introduced river roughness coefficient (2), net radiation (6) and precipitation (22) multipliers have, overall, a strong influence

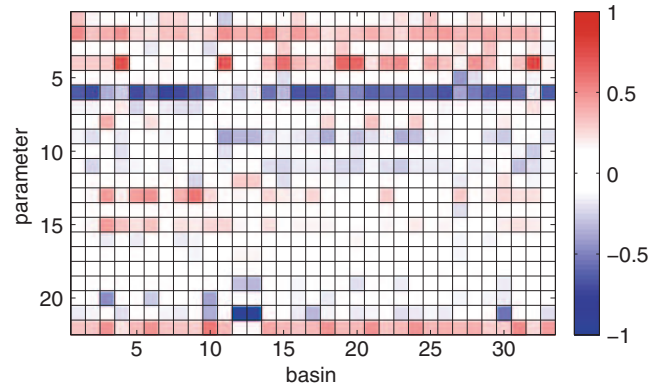


Fig. 4 Spearman's rank correlation coefficient between the calibration parameters and the mean TWS in the 33 largest river basins of the world. See Table 1 for parameter and Fig. 3 for basin names. The correlation between the mean TWS and the humid (7) and arid (8) Priestley-Taylor coefficient is shown for humid and arid regions, respectively

5 Conclusions and Outlook

The analysis of the combined model covariance matrix, as well as the performed sensitivity analysis, indicates that the correlations between the model states and parameters enable the parameter calibration by GRACE measurements. Moreover, these investigations could confirm some parameters which were identified to be most sensitive in previous studies (Güntner et al. 2007; Werth and Günthner 2009). Based on the global sensitivity analysis, a basin-wise parameter calibration seems appropriate. By performing

the regional analysis, we found that the compartments are sensitive to different model parameters. The time evolution of the parameter-state correlations indicates that the impact of GRACE changes over time. We plan to validate our calibration results by performing a calibration run for 1 year. Afterwards, the model will run for the following year, both with the standard model parameters and the calibrated values. The model states of both versions will then be compared to the GRACE observations. One can also consider independent data sets, e.g. discharge measurements, for validation. Along with the parameter uncertainties, the uncertainties of climate forcing and water use data will be included to obtain a more realistic representation of the model covariance matrix. Model improvement may also be affected by errors of the background models for other Earth system components that are used for separating TWS from the total mass signal observed by GRACE (see e.g., Forootan et al. 2014). Investigations regarding these errors will be conducted in further work.

Acknowledgements The support of the German Research Foundation (DFG) within the framework of the Special Priority Program "Mass transport and mass distribution in the system Earth" (SPP1257) under the project REGHYDRO is gratefully acknowledged.

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