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Title: **A Review of Current Best Practices and Future Directions in Assimilating GRACE/-FO Terrestrial Water Storage Data into Numerical Models**

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Reply to Anonymous Referee #2: 14 Oct 2025

General comment: In this manuscript, the authors provide a comprehensive review of current practices and future directions in assimilating terrestrial water storage (TWS) data from the GRACE and GRACE-FO missions into hydrological and land surface models. It draws on approximately 200 references to highlight advancements in frameworks like the Ensemble Kalman Filter (EnKF) and its variants, while addressing practical issues such as scale mismatches, error correlations, and applications in drought monitoring and climate trend analysis. The emphasis on geophysical corrections (e.g., glacial isostatic adjustment) and the integration of multi-sensor data (e.g., with SMAP or SWOT) provides a cohesive narrative that bridges theoretical DA with operational hydrology. The manuscript excels in its comprehensive scope and accessibility, making it a valuable resource for early-career researchers and practitioners seeking an entry point into GRACE/-FO DA. It includes detailed tables (e.g., Table 1: models that evaluated TWS; Table 2: DA frameworks) and illustrative figures (e.g., Figure 1: TWS components scheme; Figure 3: statistics from evaluations made by models).
The manuscript is timely, given the impending launch of missions like GRACE-C (2030) or NGGM and advancements in Earth System Modeling (ESM) frameworks. In general, this work is worth publishing in the Hydrology and Earth System Sciences journal, as it fills a gap in synthesizing post-GRACE-FO literature and could serve as a foundational reference for advancing standardized practices in hydrological DA, however some improvements are necessary, including deeper critical analysis and enhanced didactic elements. Some suggestions for revisions are included below and these points do not detract from its value; rather, they could enhance its rigor and relevance.

Reply: We sincerely thank you for your kind and appreciative words, as well as for the time and effort you have devoted to reviewing our work. We address your suggestions in detail below. Please note that your comments are presented in italics, our replies in standard font, and suggested changes to the manuscript are highlighted in blue.

Moderate comments: *While the manuscript is a solid synthesis, it requires moderate revisions to elevate its critical depth and utility. As a review paper, it should compile and critically evaluate the literature, identifying inconsistencies and unresolved debates. At present, the discussion is somewhat descriptive, with limited critique of methodological limitations or comparative assessments. To ensure the article meets the standards for publication, the authors must address the following critical points:*

Reply: Thank you for pointing this out. Your understanding precisely reflects what we intended with this review. We are grateful for your thoughtful ideas and hope that our revisions further clarify our intentions.

Comment 1 *Enhance your critical evaluation and gap analysis. In order to avoid a mere listing of works, I suggest to add a dedicated sub-section in Section 5 to quantify gaps. One option would be to use meta-analysis of DA performance metrics from recent studies (2020-2025).*

Reply: The meta-analysis is an interesting suggestion. However, we believe applying meta analysis to studies that use all kinds of different assumptions, error models, hydrology models and perturbations, and finally are geared towards differing applications and metrics, is a fallacy. As we suggest in this paper we need to introduce a benchmarking approach first before we can apply meta analysis to the results of different studies. We hope that this addresses the comment, which was not very clear to us. Regarding a more critical evaluation and comparison of different DA approaches, we will include a Table comparing strenghts and weaknesses of different assimilation approaches (Table 1), which you can find as part of the answer to your comment on Sub-section 3.2.

Comment 2 *Improve validation and uncertainty discussions in Section 4, since it lacks depth in metrics; mandate inclusion of quantitative benchmarks (e.g., Triple Collocation Analysis) and error propagation models. I suggest, for instance, to address how non-Gaussianity affects DA reliability, proposing solutions to make recommendations more actionable.*

Reply: We appreciate the reviewer's comment. We will expand the discussion in Section 4 to provide a more comprehensive treatment of validation metrics and uncertainty aspects. In particular, we will add an explanation of Triple Collocation, emphasizing its usefulness when multiple independent datasets are used to validate a single variable. We will also extend the section on uncertainty treatment by including a discussion on error propagation and now briefly mention error propagation models. Furthermore, we will add a statement on non-Gaussianity, explaining that non-Gaussian error distributions can degrade filter performance and validation metrics that assume Gaussianity. We now recommend employing information-theoretic measures in such cases to ensure robust validation.

We will update the text as follows:

L.562: Remotely sensed hydrological products are now widely used to validate GRACE/-FO DA simulations (Kumar et al., 2016; Zhao and Yang, 2018; Khaki et al., 2017; Jung et al., 2019). However, these datasets often differ in accuracy and consistency, making robust comparisons challenging (van Dijk et al., 2014). When multiple independent datasets are available for the same hydrological variable, triple collocation provides a way to assess the quality of each dataset without assuming that any of them is error-free (Stoffelen, 1998; Gruber et al., 2016). The method separates unpredictable measurement noise (random errors) from systematic offsets or scaling differences (calibration biases) based solely on the mutual agreement among the datasets. As such, triple collocation offers a practical solution for validation when more than two datasets are collocated in space and time and should therefore be considered a standard option.
L.573: Moreover, any preprocessing operations applied to the data (for example deseasonalizing, detrending, spatial averaging or temporal aggregation) introduce additional uncertainty which must be propagated into the final validation metrics. Error propagation models can be used to quantify the uncertainty of observational datasets by estimating how input measurement errors or retrieval assumptions propagate into derived variables. Such approaches can provide spatially explicit uncertainty estimates for each observation, thereby offering a more comprehensive view of dataset reliability than local in-situ validations alone (Dorigo et al., 2010). Neglecting these aspects can lead to overconfidence in skill estimates or misinterpretation of variance metrics, particularly when multiple data sources or preprocessing steps are involved.
An additional challenge is that both the model state distributions and even the retrieval error distributions may depart significantly from Gaussian assumptions. If validation metrics assume Gaussian error or linear relationships (e.g. RMSE, linear regression), the non-Gaussian nature of the underlying distributions may skew results or invalidate confidence statements. We therefore recommend assessing the distributional characteristics of the errors (e.g., skewness) and, where needed, applying non-Gaussian or rank-based metrics (e.g., information-theoretic scores (Kumar et al., 2018; Maina et al., 2024)) to ensure robust validation.

Comment 3 *Add didactic elements to enhance educational value, incorporate summary equations for core DA techniques in Section 3. I suggest adding schematic diagrams, such as a flowchart comparing sequential vs. smoothing DA methods, or a matrix illustrating error sources in GRACE processing.*

Reply: Thank you very much for these suggestions. This comment is also related to the remark in subsection 2.5. We will follow your recommendation and incorporate the summary equations into the flow chart of the DA concept (Figure 2 in the manuscript, see Figure 1). However, we prefer not to include an illustration of the GRACE error sources, as these are not the primary focus of our paper and have been discussed by many previous studies. Instead we will add a reference to a paper describing details of the GRACE processing and also error sources, as follows in Line 171:

These monthly gravity field estimates are typically accompanied by an error estimate of the measurement noise, provided either as formal errors or as full covariance matrices (Chen et al., 2022).

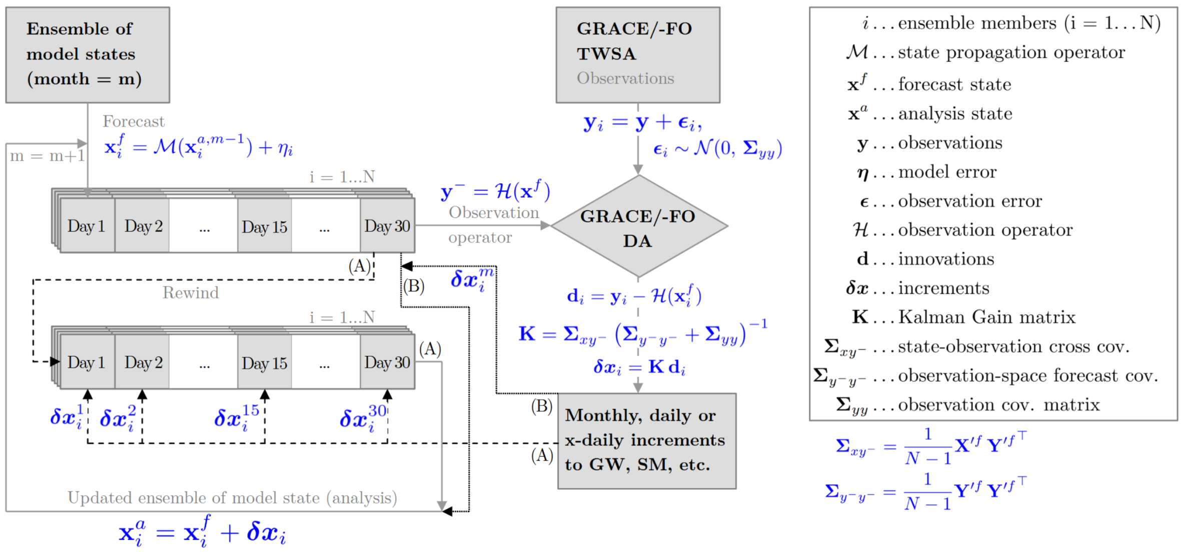

Figure 1: General concept for assimilating monthly GRACE/-FO-derived TWSA into GHMs and LSMs along with most relevant Ensemble Kalman Filter (EnKF) equations showing two options for applying the assimilation increments: After computing the increments, the model is either (A) rewound and re-run over the month with the increments $\boldsymbol{\delta x}_i^1 ... \boldsymbol{\delta x}_i^{30}$ distributed across all days, or (B) updated by applying the full monthly increment $\boldsymbol{\delta x}_i^m$ at the end of the month. Please note that the equations provided refer to the EnKF and are expressed for each ensemble member i. The Kalman Gain matrix determines the update weights based on the state and observation error covariance matrices. X'^f and Y'^f are matrices of forecast state anomalies and forecast state observation-space anomalies, respectively. Each column represents the deviation of one ensemble member from the ensemble mean. For further details on the equations for other DA algorithms, refer to the literature cited in Section 3.2 of the main manuscript.

Specific comments (Line-by-line comments):

Abstract: *1-16: The abstract is concise but could better emphasize the synthesis's novelty (e.g., "This review synthesizes over "n" studies to propose unified best practices..."). Add a sentence on key gaps identified, such as non-Gaussian challenges.*

Reply: Many thanks for your suggestions. We revise the second part of the abstract to more clearly highlight best practices and future directions, which will also implicitly address some of the identified gaps. Additionally, we will incorporate your suggestion regarding the novelty of this review. We suggest the following modification to the second part of the abstract:

In light of the upcoming launches of next-generation gravity missions and the development of increasingly sophisticated Earth system modeling frameworks, this review synthesizes insights from approximately 60 GRACE/-FO data assimilation studies in an attempt to converge to best practices. Effective assimilation strategies incorporate robust modifications of the classical ensemble Kalman filter and localization techniques, explicitly account for correlated observation errors, and address biases contained in the observations as well as those arising from model perturbations. Unmodeled processes must be carefully handled through signal separation, multisource assimilation, or removal prior to assimilation. Future directions include developing low-latency products for near-real-time assimilation, integrating enhanced and combined satellite observations, and employing machine-learning approaches for downscaling and hybrid assimilation. Collectively, these strategies provide a pathway toward more accurate, physically consistent, and operationally useful water cycle reanalyses.

Introduction: *Clarify the distinction between GRACE and GRACE-FO data continuity; reference Vishwakarma et al. (2021) for gap-filling techniques. I suggest to add a simple timeline figure of GRACE missions to make the historical context more didactic.*

Reply: We thank the reviewer for highlighting the importance of clarifying GRACE and GRACE-FO continuity. In the revised manuscript, we now explicitly discuss the observational gap and reference existing gap-filling methods, including hydrological models, autoregressive approaches, and machine learning reconstructions. We prefer to do this in Section 2 rather than in the introduction, so that the introduction remains concise and focused on only the most relevant information. We also note that we could not identify any peer-reviewed publication by Vishwakarma et al. (2021) that addresses the GRACE–GRACE-FO gap; their work appears restricted to downscaling applications. Unfortunatley, we were not able to find the reference Vishwakarma et al. (2021). We will modify the beginning of Section 2.2 to:

The GRACE satellite mission (Tapley et al., 2004) monitored global TWS changes (Wahr et al., 1998) from 2002 to 2017, with its follow-on mission GRACE-FO, launched in 2018 (Landerer et al., 2020), continuing these observations. TWS changes are an essential climate variable reflecting the impact of global climate change on water resources (Rodell and Reager, 2023).

Furthermore, we will add details regarding gap filling techniques:

Although GRACE and GRACE-FO provide a largely continuous record of TWSA, there is an observational gap between the missions of almost one year. Several studies have addressed this gap using different methods, including physically based hydrological models (Zhang et al., 2022), interpolation and statistical approaches such as singular spectrum analysis (SSA) and autoregressive (AR) models (Lecomte et al., 2024; Lenczuk et al., 2022), and machine learning techniques including convolutional or recurrent neural networks (Uz et al., 2022; Mo et al., 2022). These techniques allow reconstruction of TWSA during the gap while preserving both seasonal cycles and long-term trends.

Sections 2 to 7:

Sub-section 2.3 *Expand on geophysical corrections with an equation for leakage error correction.*

Reply: In l. 223-225, we write: "To account for leakage globally before DA, rescaling is commonly applied, which means that TWSA scale factors are estimated from hydrological model output, which in turn creates another source of uncertainty."
In fact, there are several approached how to restore the GRACE/-FO signal due to signal damping in the filtering process. We will reformulated the sentence in l. 223-225 to:

To account for leakage before DA, several approaches are available such as estimated from hydrological model output, which in turn creates another source of uncertainty, or from data-driven approaches (see Sect. 2.2 for details).

Furthermore, we will add the named approaches in l. 181 of the manuscript to provide a fuller picture of the available methods:

To account for spatial leakage effects, several methods have been developed that attempt to restore the lost signal in GRACE/-FO data. Commonly used approaches that depend on hydrological model outputs are the multiplicative approach by Longuevergne et al. (2010), the additive approach by Klees et al. (2007), the grid factor scaling approach by Landerer and Swenson (2012), and the unconstrained forward modeling approach by Chen et al. (2015). Vishwakarma et al. (2017) developed a data-driven approach to overcome the dependency on hydrological models and their associated uncertainties.

It is beyond the scope of this paper, to provide equations for all of the named approaches and the reader is referred to the cited literature for this purpose.

Sub-section 2.4 *Include a recent reference (Gerdener et al., 2024) on GRACE/-FO data uncertainties. Propose a schematic diagram illustrating the GRACE processing chain from raw measurements to TWS anomalies.*

Reply: Thanks, we included the reference for the GRACE/-FO data uncertainties in this section and added a sentence. The processing chain is indeed an interesting part. However, most systems include level-2 measurement and only few use level-1 measurement but none uses raw measurements. In addition, the processing, e.g., from level 2 spherical harmonic to level-3 TWS anomalies changes from assimilation system to assimilation system. Due to these reasons and due to the fact that figures of processing schemes already widely exist, we would like to refer to existing illustrations here and keep the description of the levels that we provided in the section of GRACE/-FO data products as is. These illustrations contain detailed information of, for example, processing from level 0 raw measurements to level 2 spherical harmonics[1 2] (e.g., Ferreira et al., 2023; Gerdener, 2024).

Sub-section 2.5 *Although the article is a review paper on the application of data assimilation techniques, mainly from the Kalman filter family, I recommend at least adding the basic EnKF equations for accessibility.*

Reply: We appreciate your suggestions on this topic! Indeed this comment was also made by the other reviewer. As we prefer to keep equations out of the main text, and it is not possible to include equations for all types of filters, we have decided to present them in a figure. We plan to add the key equations to the current Figure 2 of the manuscript (see Figure 1), making terms such as 'innovations' and 'increments' more accessible to the reader.

Sub-section 3.2 *I strongly suggest a table or matrix comparing DA methods' computational costs and assumptions.*

Reply: Many thanks for this suggestion, which we are happy to follow. We will add a table to this section to clarify the computational costs, relative strengths, and limitations of the DA methods discussed (Table 1):

[1] `https://www2.csr.utexas.edu/grace/asdp.html`, last accessed 11.11.25

[2] `https://www.gfz.de/en/section/global-geomonitoring-and-gravity-field/projects/closed-projects/grace-gravity-recovery-and-climate-experiment-mission/grace-products`, describe how TWS anomaly grid is derived from the level 2 spherical harmonics (e.g., Feng, 2019) or provide an overview of the common levels (within levels 0 to 3) plus integration of other approaches for example, assimilation[3], last accessed 11.11.25

Table 1: Comparison of DA methods and ensemble tuning techniques commonly applied in GRACE/GRACE-FO DA cases. Computational cost is rated qualitatively: ★☆☆☆☆ (low), ★★☆☆☆ (moderate), ★★★☆☆ (moderate–high), ★★★★☆ (high), ★★★★★ (very high).

Method / Technique	**Computational Cost**	**Key Assumptions**	**Strengths**	**Limitations / Notes**
EnKF	★★☆☆☆ (moderate)	Assumes Gaussian unbiased errors; ensemble approximates covariance	Efficient for large-scale hydrology; real-time capable; uncertainty quantification	Sampling errors for small ensembles; prone to ensemble collapse; requires localization and inflation
EnKS	★★★☆☆ (moderate–high)	Same as EnKF; assumes temporal error correlation over smoothing window	Improved temporal consistency; suitable for monthly GRACE/-FO assimilation windows	Higher memory and computational cost; retrospective only
Square-root filters (ETKF, EAKF, ESTKF)	★★☆☆☆ (moderate)	Same Gaussian assumptions as EnKF	Uncertainty quantification, reduced sampling noise; improved numerical stability; smaller ensembles possible	Still requires localization and inflation; additional linear algebra steps
Particle Filters / Particle Smoothers	★★★★★ (very high)	No Gaussian assumption; fully general Bayesian formulation	Handles nonlinear and non-Gaussian dynamics; accommodates multimodal states	Computationally infeasible for global LSMs; particle degeneracy unless many particles are used
Hybrid Machine Learning–DA	★☆☆☆☆ – ★★★☆☆ (variable)	Requires representative training data; assumes model transferability	Can reduce structural model error; enables downscaling or emulation; useful where physics are weak	Can generalize poorly; GRACE/-FO record is short; physical consistency may weaken
Localization (covariance or domain)	★★☆☆☆ – ★★★☆☆	Forecast error correlations decay with distance	Mitigates spurious long-range correlations; essential for small ensembles; improves stability in GRACE/-FO DA	Choice of radius is subjective; too strong localization distorts updates; often combined with inflation
Covariance Inflation	★☆☆☆☆ (low)	Forecast ensemble under-dispersion can be corrected multiplicatively or additively	Prevents filter divergence; widely used in GRACE/-FO DA; prevents underestimation of forecast model error covariance	Over-inflation causes noise or instability; parameters often tuned empirically
Adaptive Inflation	★★☆☆☆ (moderate)	Innovation statistics correspond to correct ensemble spread	Online tuning reduces need for offline sensitivity tests; improves filter robustness	Additional computation; may react poorly to biased observations or large model error

Sub-section 6.1 *Strengthen ML discussion with a hybrid DA-ML schematic (e.g., EnKF with LSTM for error modeling).*

Reply: Indeed, this is an important point, which was missing in the manuscript. Many thanks for this suggestion! We plan to add to Section 6.1 the following text and Figure:

Recent years have seen substantial progress in applying ML within DA systems for numerical models, particularly in geophysical applications such as improving regional climate simulations (Bocquet, 2023; He et al., 2023; Keller and Potthast, 2024). GRACE/GRACE-FO DA frameworks can benefit from ML at several stages of the assimilation workflow (Figure 2). As described above, ML can support observation preprocessing, including gap filling and spatial downscaling of coarse TWSA fields. ML can potentially act as a surrogate observation operator and might also support the model update step by learning hydrologically meaningful distributions of DA increments across storage compartments. More intrusive uses involve learning from the state corrections produced during assimilation, enabling targeted model-error correction at each forecast step (Arcucci et al., 2021). Finally, the DA algorithms themselves (e.g., EnKF variants) can benefit from ML – for instance, by automatically correcting the ensemble spread through ML-based adaptive inflation or improving covariance structure by ML-based localization schemes – and may even be replaced by ML architectures designed to emulate full sequential filtering. However, these potential benefits need to be balanced against the substantial computational cost of training such models. In several meteorological applications, the training effort can exceed the runtime savings unless transfer learning strategies are used to adapt pre-trained models to new domains or conditions. Similar considerations are expected for GRACE/GRACE-FO DA, where the limited length of the observational record poses additional challenges for generating suitable training data.

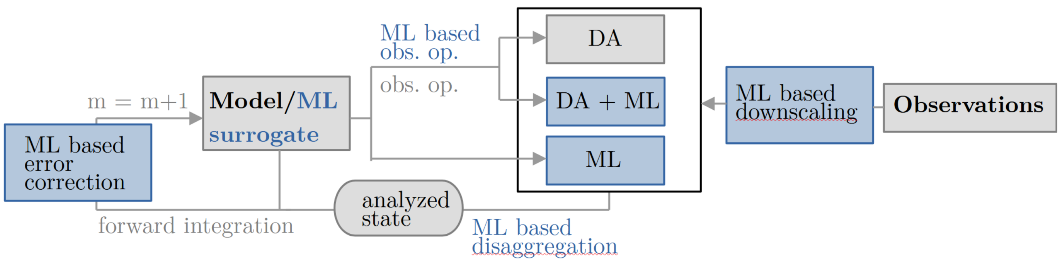

Figure 2: Workflow of a data assimilation framework with potential machine-learning augmentations highlighted in blue; note that these enhancements represent alternative components of the workflow, and it is generally not meaningful to apply ML at all components simultaneously.

References and General: *Ensure all citations are up-to-date, specially from 2020-2025. The manuscript could benefit from an appendix with a glossary of DA terms for non-experts.*

Reply: This is a very good idea! We will add a glossary to the appendix (see Table below). Furthermore, we added some references regarding gap filling approaches and the following recent studies that focus on GRACE/-FO DA:
Retegui-Schiettekatte et al. (2025)
Arciniega-Esparza et al. (2025)

Table 2: Glossary of key data assimilation terms used in this study.

Term / Acronym	**Definition**
3D-Var	Three-dimensional variational data assimilation: adjusts the model state at a single time step by minimizing a cost function combining background and observations.
4D-Var	Four-dimensional variational data assimilation: adjusts initial conditions over a time window to match observations distributed in time, minimizing a cost function subject to model dynamics.
Analysis state	The model state after assimilation, obtained by optimally combining the background state and observations.
Background state	The model state prior to assimilation, representing the best estimate of the system before incorporating observations.
Bias correction	Adjustments applied to model or observations to remove systematic differences.
DA	Data Assimilation: combining model predictions and observations while accounting for uncertainties.
EnKF	Ensemble Kalman Filter: sequential DA using an ensemble to estimate state and error covariances.
EnKS	Ensemble Kalman Smoother: updates states over a time window using past and future observations to improve earlier estimates. For GRACE/GRACE-FO TWSA assimilation, the smoothing window is typically one month, meaning the monthly observation is used to redistribute the increment across the days of that month for improved temporal consistency.
Error covariance matrix	Represents uncertainties in the background model and/or observations; used to weight contributions in DA.
Filter	Sequential DA method updating the state at observation times.
Hybrid methods	Data assimilation approaches combining ensemble-based and variational techniques to leverage the advantages of both.
Increment	Adjustment applied to the model state computed by the DA algorithm.
Innovation	Difference between observations and model-predicted observations.
Inflation	A technique to artificially increase the ensemble spread in sequential DA, compensating for underestimation of uncertainties due to finite ensemble size or model errors.
Localization	Limits the influence of observations to nearby model grid points to reduce spurious correlations.
Observation operator (H)	Maps model state variables to observation space for comparison with observations.
Particle Filter (PF)	Nonlinear, non-Gaussian DA method using a weighted ensemble (particles) to represent the probability distribution of the state.
Rewind / Re-run	Strategy distributing monthly increments across previous days to improve temporal consistency.
Smoother	DA method updating states over a time window using multiple observations.

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