Interactive comment on "Unsaturated zone model complexity for the assimilation of evapotranspiration rates in groundwater modeling" *by* Simone Gelsinari et al.

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Response to Anonymous Referee 1

We thank the Reviewer for their detailed analysis of the manuscript. We disagree with a number of the points raised in the review in relation to the presentation of the manuscript, the model conceptualization and the data assimilation algorithm. Details on these aspects of the manuscript are provided below, with the Reviewer's comments in italic.

1 - Paper Presentation

Explaining what kind of parameters your model uses is not particularly helpful if you are not providing the governing equation(s) of your UZM. After skimming Gelsinari et al. (2020) (recommended reading 'for a detailed description') I could also not locate the governing equations anywhere in the original publication. If you develop a new method, at least show us exactly what you are doing mathematically. Section 2.2.2: The explanation of SWAP is great, but again, show us how your UnSAT-UZM functions to at least the same degree of detail (and this does not mean explaining what it does, but providing the equations).

The UnSAT unsaturated zone model (UZM) was presented in Gelsinari et al. (2020), with the equations reported in its supplemental material. We do not think that including the UnSAT model description in this manuscript or in its supporting information is needed. Please also be aware that the submission system does not allow manuscripts with too much overlap with published papers. However, we will revise the manuscript to be more specific on where to find these equations. We will also revise the description of the model to clarify the meaning of the parameters listed in the manuscript.

Section 2.2.3: First off, normally FloPy generates the entire model input for MODFLOW (not just Kh and Sy as well as the model discretization), so just say that you use the MODFLOW-Python interface FloPy to create the model – that's much clearer. Also, provide the MODFLOW input files, because the current information about the model parameterization is sparse at best, and choices made in the other packages (particularly the solver) can severely affect the fidelity of the results obtained.

We agree on the fact that FloPy generates the entire groundwater model. We will add

the suggested sentence "FloPy was used to generate the model".

In addition, choosing eight-day time steps for groundwater models is certainly not conventional. There is no real reason why you should reduce the MODFLOW time step size to the resolution of the CMRSET data set. The CMRSET ET estimates do not serve as input for MODFLOW (your UZM predictions, available at a finer temporal resolution, already do this job). Even if you only had inputs on this temporal resolution, MODFLOW allows the definition of coarsely-resolved stress periods (during which forcings are either assumed blockwise-constant or are interpolated) subdivided by timesteps of a finer temporal resolution.

The 8-day frequency, albeit unusual for groundwater applications, is the most efficient time step for the assimilation framework, as the filter would update the state variable of MODFLOW (i.e. heads) with this frequency. This minimises the required input/output phase between the filter (to which the CMRSET is an input) and the model, which is one of the most time consuming tasks of the entire process.

The Reviewer further states that a finer temporal resolution for the groundwater model would not have greater computational time in the present configuration. Adding that: ... If your model takes a suspiciously long time to solve, this might be evidence that the solution of MODFLOW's iterative solver is unstable, which should set off alarm bells concerning the model design. This is something you could check by analyzing the list .LST (list) file, looking at the residuals and the convergence. Also, you are definitely NOT on a regional scale for groundwater models: your model domain is only 1 km by 3 km.

We acknowledge that, at this scale, refining the temporal resolution of the groundwater

model is possible. However, the model is set-up for application at the regional scale. This justifies the choice of the time step of the coupled models to match the frequency of the assimilated observation. Additionally, because observations of water table levels are available approximately every 3-4 weeks, the 8-days step can be considered a fine temporal resolution. The long time taken by the simulation is not due to the issues with the convergence of the iterative procedure to solve the equations. The MODFLOW solver (CONJUGATE-GRADIENT SOLUTION PACKAGE, VERSION 7, 5/2/2005) usually takes less than a second (with residuals below 0.05

Are you using the MODFLOW-Sy also as the specific yield for Configuration-2? If so, why do you call it MODFLOW-Sy in the table? Is Sy the same for both soil layers? Also, the reference to section 2.3 is nonsense – there is not a single mention of Sy in this entire section.

Specific yield (Sy) is a MODFLOW parameter that is independently used and calibrated in Configuration-1 and Configuration-2. The second question is unclear, please reformulate. There are not two soil layers for the MODFLOW model, as explained in line 171-172 "...applied to domain of 1 x 5 cells of 1 km2 each, and a single vertical unconfined layer" Sy is then mentioned in the table of section 2.3; however, we agree that is not further explained in the section. We will amend this.

The reviewer makes a number of remarks on Figure 3

We agree with the reviewer on better presenting Figure 3, and we will modify it accordingly in the revised version of the manuscript.

You never mention at what tables you fixed your prescribed head boundaries. Also, you should not reference section 3.1 (part of the results section). You have to explain

the model setup in the Methods section, not refer to the results section to complete the picture. Clarify what you mean by saying you changed the boundaries to obtain 'more shallow water tables': Shallower in terms of distance from the surface (=increased WT) or a shallower water body (= decreased WT)?

We thank the Reviewer for noting this. We described why we selected the constant head boundaries, but missed to report the actual value (i.e -3.5 m below the surface); this will be added in the revised version of the manuscript. We will also modify the text to avoid referencing to following sections in the methods. In the entire manuscript, we always referred to shallow water table being a water table closer to the surface. We will make this clear in the revised manuscript.

If your UnSAT-UZM is discretized into layers anyways, why can't you represent the sediment heterogeneity the same way as the SWAP-UZM? This limitation seems poorly justified and reduces the comparability between the two approaches.Elaborate on why you had to make this distinction

The conceptual UnSAT UZM becomes unstable when accounting for sharp vertical changes in the soil parameterizations. Therefore, we accounted for the decrease in the hydraulic conductivity across the soil column. These details were not clearly stated and will be added in the revised manuscript.

The reviewer requests that we clarify what we mean by "interdependence between WT and actual ET".

In many ecosystems where the roots can reach the capillary fringe, transpiration rates depend on groundwater levels; in turn, water table depths in these situations

are related to the transpiration rates. This means that the link between the water table dynamics and transpiration must be correctly modeled. This relationship has been shown in many studies, both experimentally (Vincke and Thiry, 2008; Benyon et al., 2006, Marchionni et al., 2019) and using numerical models (Loheide et al., WRR 2005). In many areas in the southern part of Australia, trees can grow roots to several meters to tap the capillary fringe at large depths. An often used reference for eucalyptus plantations, for example, is that the roots can use groundwater when the water table is about 6 m (Benyon et al., 2006); however, trees have been observed to use groundwater at very different depths, reaching more than 20 m below ground (Eamus et al, 2015). We will provide more details on this in the revised version of the manuscript to strengthen the justification for the application of the models and the assimilation procedure that we used.

Throughout the manuscript we deal with this concept in:

Abstract: "..ET rates are assimilated because they have been shown to be related to the groundwater table dynamics.."

Introduction: "...Because ET is a function of the soil water content within the root zone, as the root water uptake is distributed along the entire root system, improving ET estimates, by means of a detailed modeling of the soil water transport, can lead to better simulation of recharge and WT dynamics. This is particularly important when the WT is within the reach of the roots, as it is common in Australian semi-arid catchments..."

Study area description: "Because in the area more than 90these plantations have been shown to have direct access to groundwater (Benyon and Doody, 2004)."

Calibration section: "...For both configurations, attempting to assimilate ET fluxes, without reproducing the interdependence between WT and actual ET, yielded poor filter performances." and again by introducing a multi objective function which calibrates specifically on the two quantities.

And exposed in the "Results and Discussion" and "Conclusion" section as a fundamental step for the ET data assimilation.

We are convinced this should be enough explanation for the concept. However, we are available to provide more details.

To verify the spread and accuracy of the ensemble, a number of statistical variables, originally developed for numerical weather prediction by Talagrand et al. (1997), were calculated on the ensemble population." What kind of 'statistical variables' did you calculate? Why did you calculate them? Right now this sentence provides as much information as writing "and then we did some unspecified math.

We agree that more detail are needed on this aspect. We calculated the ensemble skill (esnk), ensemble spread (ensp) and mean squared error (mse) (Talagrand et al. 1997; De Lannoy et al., 2006) for the ET values and applied them to verify the ensemble as in Gelsinari et al. (2020). We will clarify this in the revised version of the manuscript.

2 - Model Choice, Conceptualization, and Set-up

The Reviewer asks why we did not use HydroGeoSphere, or the MODFLOW EVT or UZF packages.

Despite its limitations, MODFLOW is a very commonly used model, particularly in groundwater management. This project was developed to underpin and support existing MODFLOW groundwater management models in the South East and many other parts of Australia. We therefore focused on which conceptualisation of the unsaturated zone is most appropriate to couple with MODFLOW. We will add details on this in the revised manuscript to justify the selection of the model.

We did not use the MODFLOW EVT or the ETS packages as they do not account for more complex relationships between depth to groundwater and both evapotranspiration and recharge (Doble and Crosbie, 2017). The UZF1 package, which is already coupled to MODFLOW, would be an alternative to SWAP. However, SWAP solves the full Richards equation, while UZF1 solves a kinematic wave approximation of the Richards equation. Also, SWAP is considered a better model for the soil-water-vegetation interaction (Vereecken et al., 2016), an important aspect when modeling vegetated areas. SWAP combines detailed modules on soil water flow, root water extraction, vegetation development and evapotranspiration. The model has been extensively applied in scientific research (https://swap.wur.nl/).

Your groundwater model is highly unrealistic, its coupling with the UZM likely extremely exaggerated (as hinted by the need to calibrate both parts to avoid 'poor filter performance'), which invalidates the results you obtain and the conclusions you draw from it.

We disagree with this statement and we address all the remarks the Reviewer made in relation to this issue below.

...with the groundwater model, I take issue with the decision to resolve a 3 km by 1

km model domain with only three numerical cells (plus two prescribed-head boundary cells). This has a number of highly questionable consequences: If you wish to resolve a hydrogeological depression, choosing such a coarse spatial resolution severely affects which drawdown curve you obtain.

The scope of this manuscript is not to resolve a hydrogeological depression in space. The observation of water table levels presented are at a single location. We recognize that the model conceptualization phase is a fundamental aspect of any numerical simulation. The simple model domain is a result of numerical experiments which have shown us how it is possible to obtain similar water table dynamics with both a fine (20 cells in the x-axis) and coarse (5 cells in the x-axis) model domain. Figure 1 at the end of this document shows the water table fluctuation, calculated with Configuration-1, in the cell of the two domains simulating a similar location in the same study area. It is worth to say that the run-time for the fine set-up is roughly 5 times larger than for the coarse set-up. If we were to resolve the cone of depression induced by the root transpiration we would have certainly decided for a different conceptualization.

We purposely did not use a very fine resolution because (1) the MODIS-CMRSET data are already at a 1 km resolution and (2) the intention is to apply this work at a regional scale, thus prohibiting very small cell sizes. The work is the first step toward the application of the EnKF to large-scale groundwater modelling.

The Reviewer says that with the given boundary conditions, "In essence, you artificially prevent that any other external influence (say, regional irrigation water extraction during summer, regional water table fluctuations due to seasonal variations in precipitation and ET, etc.)"

The location of the study is in the centre of a forestry block, more than two kilometres from any groundwater extraction, and was originally selected for a previous study to specifically look at the impacts of forestry on groundwater (Benyon et al., 2006).

Groundwater use (not total ET, but ET from a groundwater source) by forestry (Pinus radiata and Eucalyptus globulus) for this region, where the water table was less than 6 m below the surface (and soils were light to medium textured and groundwater was not saline) was estimated by Benyon et al. (2006) to be on average 435 ML/yr (range 108–670 ML/yr) for a 1 km by 1 km fully forested cell. This exceeds by around 2 orders of magnitude the maximum groundwater extraction rate from a single bore for the region, albeit on a diffuse scale rather than point scale. Working on the assumption that there is not likely to be more than one or two high extraction bores in a 1 km square area, water use by forestry is seen to be significant. For this reason, and from personal communication with water managers in the region, it is a valid assumption that the impact of recharge and transpiration from forestry on groundwater would far exceed the impacts of extraction through pumping and other temporal variations.

In an uncalibrated, coupled model the influence of actual ET on the water table would be likely negligible (there is a reason why hydrogeologists often neglect the UZ).

Where groundwater is deep, this is a reasonable assumption. ET is exclusively from infiltrated rainfall in the unsaturated zone, and not supplied by the groundwater. Most of the surface processes are damped by the large lag time between infiltration and recharge. However, where groundwater is within plant rooting zones, more specifically lower than 10 m from the surface with a range of 6 m 20 m (Crosbie et al., 2015, Benyon et al., 2006), particularly in semi-arid areas, ET can have a significant effect on the water table, as demonstrated in Vincke and Thiry (2008), Benyon et al. (2006) and Eamus et al. (2015)

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Since you dynamically readjust the resolution of your UZM: Do you account for hysteresis effects? How thick are these layers? Are you assuming the water tables as blockwise-constant or do you interpolate between them?

We do not account for soil water hysteresis effects, as this has a minor effect on regional groundwater recharge simulation. The layer thickness for the UnSAT model is fixed to 10 cm. We assume that the water table is measured at the centre of a model cell and blockwise-constant.

why is the root depth so dramatically different between the two configurations? This should be a system property, and as such be constant between the two configurations. It makes no sense to assume two different root depths if you want to compare the two models.

As the two UZM are conceptually different, they dissimilarly account for this parameter. Specifically, as UnSAT does not simulate the capillary fringe, the direct extraction from groundwater is possible with a root depth that allows roots to reach the water table. Therefore the root depth in UnSAT is larger than for SWAP. We will add a comment on this in the revised version of the manuscript.

3 - Data Assimilation

The Reviewer makes a number of remarks regarding the data assimilation algorithm, which can be summarized as follows:

The Reviewer states that we may not have understood the theoretical foundations of the DA algorithm because we state that the EnKF was used because of its ability to deal with highly non-linear systems, and encourages us to revisit the derivation of the EnKF.

Evensen (1994) developed the EnKF to deal with nonlinear systems, by replacing the propagation of the error covariance in the Extended Kalman Filter by an ensemble-based calculation. He stated in the abstract of his paper: "The proposed method can therefore be used with realistic nonlinear ocean models on large domains on existing computers". The difference between the Discrete Kalman Filter (as originally derived for linear systems by Kalman), the Extended Kalman Filter and the Ensemble Kalman Filter is the calculation of the error covariance. The only one in this family of filters that does have a derivation is the original DKF.

The Reviewer states that the EnKF can only use nonlinear models because it fits a Gaussian distribution to the ensemble after the forecast.

The EnKF does not fit any distributions, it updates state variables. Also, a filter does not use a model, it is the model that uses the filter.

The Reviewer suggests using the particle filter.

We have experience with Particle Filters, and our experience is that a much larger ensemble size is required than for the EnKF, which is one of the reasons why we decided to use the latter for this study.

The Reviewer argues that we should not justify the ensemble size with examples from literature.

Enough papers have been published on this issue. For soil moisture assimilation, it has been shown that in land surface model data assimilation, an ensemble size of 12 (Yin et al., 2015) or even 10 (Kumar et al., 2008) is sufficient. Based on our experience with models of this level of complexity, an ensemble size of 32 is more than sufficient.

The Reviewer argues that the assimilated variable should be in the state vector and that the observation matrix should contain zeros and ones.

The main advantage of the EnKF is the possibility of assimilating proxies of state variables that are nonlinearly related to the state variables. Examples are the assimilation of brightness temperatures or radar backscatter values into land surface models to update the soil moisture simulations, or the assimilation of streamflow into flood forecasting models to update the modeled soil water content.

The Reviewer states that parameters should not be disturbed when generating the ensemble.

The essence of an ensemble is that all members have different properties. Reichle et al. (2002), who introduced the EnKF to the hydrological sciences, explicitly state that parameters can be disturbed or that even different models can be used to estimate the error covariance.

The Reviewer refers to Hendricks-Franssen and Kinzelbach (2008) for an explanation

on how to update parameters and states.

The main point of the paper that is referred to is error covariance inflation, which is necessary because the ensemble is inadequately generated and over time becomes too narrow. Our approach explicitly avoids this problem.

The Reviewer states that figure 10 is comical, and that there is something wrong with the DA algorithm, b ecause the soil moisture does not change while the AET does change, and that this means that the ensemble has collapsed.

The AET is the integrated response of the root system. The DA system has lowered or increased the water table level, and thus layers are added to or removed from the unsaturated zone. This will modify the modeled AET. This lowering or raising of the WT means that the ensemble has not collapsed. This result does not mean that the DA system doesn't work, but, conversely, it proves that it does work.

Furthermore, here the Reviewer states that the ensemble has collapsed. Towards the end of the review, the statement is made that the settings (through selective parameter perturbation) seem to have been deliberately designed to inflate the WT uncertainty disproportionally, amplifying the Kalman update through the cross-covariances. These comments are contradictory.

4 - Final remarks

With this document we are expressing our disagreement with the reviewer's remarks about the methods adopted in the manuscript, reinforcing the appropriateness of our

choices and the theory underpinning the experiments. However, in this reply we are not going to provide a response to the remarks on the "Results and Discussion" and "Conclusion" sections, as we have shown the Reviewer is basing these comments on inexact assumptions.

In general, the tone of the review and the use of words such as "fraudulent", "fudging", "comical", etc., are not appropriate for a review for a scientific journal. Certainly not for a review in the public domain. It is also not appropriate to state that the authors do not understand the methods that they are using, while is the reviewer that appears not to have understood the applied methods.

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Water table fluctuation at the centroidal cell of the domain for Configuration-1 after calibration. The simulation is based on real forcing inputs. The "Coarse" resolution is a 5 X 1 cell domain, same as the one used for the experiment in this paper. The "Fine" resolution is a 20 X 1 cell domain.
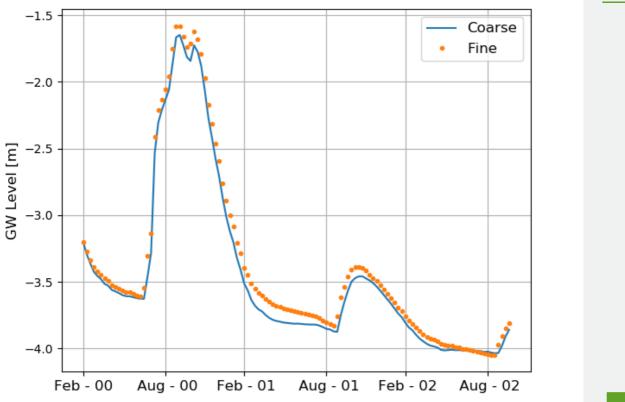

Fig. 1.