Response to the Referee for article hess-2013-463

Note: The text in black is the original comments from the referee, and the text in blue, headed with "Reply", is the response from the authors.

General comment

This is a re-review of the paper. I will focus on the theory, not the results. The theory and implementation of the EnKF for joint parameter and state estimation is questionable - even though it is based on previous work by others, the methodology is incorrect and statistically invalid. Of course the results of this (and other papers that use this methodology) are affected by this wrong implementation.

Reply: We appreciate the reviewer for a few useful suggestions to ameliorate the paper. We have incorporated these suggestions in the study and revised the manuscript accordingly. Although the methodology used in this study is not perfect, we argue it is valid and effective for the steamflow simulations/predictions at ungauged locations. Similar methodologies have already been successfully applied by a number of scientists in hydrology and hydrogeology. In this response, moreover, we provided a simple case to validate the methodology (reply to comment 10). Please see point-by-point replies below.

Review Comment 1

Equation 2: You use Q_t to denote the covariance matrix of the model error. This might be confusing because "Q" is often used to denote streamflow - whereas in this case you use it for the states. Would suggest to use another symbol.

Reply: In this revised manuscript, we used W to replace Q in equation (2). Thanks.

Review Comment 2

With equation (2) an immediate question that pops up is: how did you decide which covariance matrix of Q to use? Problem is that you perturb different states - each of those states has a different magnitude and time behavior. How do you know that your state perturbations are realistic when measured in the output (streamflow) space? This constitutes a serious problem. That is why I strongly recommend to do the perturbation in the streamflow space and then to compute the analysis streamflow which you then use to compute the corresponding analysis states. It is much easier to define the model error in the streamflow space rather than the state space! For instance is your model error heteroscedastic? Does it increase with simulated flow level? When done directly in the state space this is very difficult to tune and derive an appropriate covariance matrix that can do this. You can circumvent this by problem doing the Kalman analysis in the streamflow space, and then to derive the corresponding analysis states.

Reply: We agree with the reviewer on the perturbation. Equation (2) is written in a general form to represent the forecast step with representative errors (i.e., ω_t) for state and fluxes. In implementation, we only perturbed the streamflow and soil moisture (Note precipitation as an input is also perturbed). SWAT modeling error generally increases with the level of simulated streamflow (Clark et al., 2008; Xie and Zhang, 2010, 2013).

Soil moisture is a very active variable in controlling runoff generation and other hydrological processes. It is usually perturbed to reflect modeling uncertainties and thereby produce more reasonable uncertainty for streamflow simulation (Chen et al., 2008; Crow and Ryu, 2009).

The general form of equation (2) may confuse the reviewer. Thus we provided a few more explanations and descriptions (line 12-15, page 7; line 14-17, page 14).

Review Comment 3

The kernel smoothing technique and state augmention method for parameter estimation. Does this converge to the "correct" posterior target distribution. Vrugt et al. (2013) demonstrate it does not and discusses why this is the case. I consider this a serious flaw in the current work (and previous work by others this work is based on). Also, the settings for the smoothing and shrinkage factor, etc. strongly affect the results - and different settings are required for different problems. This is not desirable. A universal method is available that does not rely on subjective algorithmic parameter values and incorrect theory.

Reply: Thanks for providing the information about discussions by *Vrugt et al.* (*2013*). We didn't find the associated literature even after visiting the publication list at Jasper Vrugt's homepage. Despite the potential different opinions by *Vrugt et al.*, we argue that the state augmentation method and the kernel smoothing technique are capable of approaching the optimal/suboptimal (or true) estimates of parameters. Our argument is based on following three reasons:

(1) Many researchers have successfully applied the state augmentation method to retrieve model parameters, including the cases in hydrology (e.g., Moradkhani et al., 2005; Wang et al., 2009; Xie and Zhang, 2010, 2013; Tran et al., 2014), hydrogeology (e.g., Chen and Zhang, 2006; Liu et al., 2008; Xue and Zhang, 2014), and ecology (e.g., Chen et al., 2008);

(2) The state augmentation method still relies on the basic tenet of data assimilation: spreading information from easily-observed variables to model variables (and parameters) that are difficult to be observed and in some way connected to the observations (Reichle, 2008). In this case, model parameters are assumed as an conceptual extension and they could vary slowly with time, in response to changes of environmental forcing inputs (Liu and Gupta, 2007);

And (3) for the kernel smoothing technique, the smoothing factor α in equation (3) is the only one factor that is subject to prescription prior to applications (the shrinkage factor h can be estimated by $\sqrt{1-\alpha^2}$). Although the setting for the smoothing factor partly depends on trial and error experimentation, it generally ranges in [0.95, 0.99].The kernel smoothing is just one of the techniques used to perturb parameters and thereby avoid ensemble shrinkage in data assimilation (Moradkhani et al., 2005). One can use another alternative technique, i.e., the random walk scheme (Wang et al., 2009).

As the reviewer mentioned, Vrugt et al. (2013) may have different opinions on the state augmentation method and the kernel smoothing technique. We have emailed Dr. Vrugt, and expect to make further discussions on the methods in future work. It is interesting to reveal their robustness and appropriateness for state and parameter estimation under different hydrological models. In this study, we focused on streamflow prediction at ungauged locations using a data assimilation scheme (i.e., PU_EnKF). There are optional and capable methods, such as the Particle-DREAM method (Vrugt et al., 2013), the Maximum Likelihood Ensemble Filter with state augmentation scheme (Tran et al., 2014). It will be an encouraging attempt to implement these methods with distributed hydrological models for hydrological predictions in ungauged basins. A brief discussion on this point was incorporated (line 3-5, page 6; line 14 – 17, page 21).

Review Comment 4

Equation (7) - the model states are updated using the standard Kalman analysis equation. It would be much more productive however to use an alternative scheme that takes into consideration how much water is originating from what tank. For instance, during high flows, it does not make sense to update the groundwater (baseflow) reservoir, and vice versa during low flows it would not be productive to update the quick flow reservoirs. Instead, if one first computes the contribution of each constituent component of the discharge then one can use this information to appropriately update (according to percentage contribution) the respective reservoirs where these fluxes originate from. For instance, during low flow, the large majority of the streamflow will constitute baseflow - for instance 90%, the other 10% can come from the other thanks. Then, 90% of the difference between the analysis discharge and forecasted discharge should be attributed to the slow flow tank, and not an equal distribution among the tanks. This will significantly enhance the implementation of the filter and the quality of the results as water is entered into the right tanks.

Reply: It is a good idea. We incorporated it in this study and re-did all cases (Figure 2-6 were updated). Specifically, the model states are divided into three groups: (1) quick water storage regarding surface runoff (marked with QW in Table 2), (2) slow water storage associated with baseflow and groundwater flow and soil moisture (marked with SW), and (3) river channel storage and flow (marked with CW). When precipitation occurs at the time steps, the states of the quick water storage are updated; otherwise, the states of the slow water storage are updated. The states regarding the river channel storage and flow are updated at every time step. In this way, the streamflow prediction is improved to some degree comparing with the implementation of updating all states at every time step (Figure 2 and 3 in the manuscript). Necessary description is presented in the manuscript (line 26 -27, page 11; line 1-3, page 12; line 4- 8, page 16).

Review Comment 5

5) Equation (8) --> sentence just prior "....these variables...". which variable are referred to? It seems unrealistic to describe rainfall errors with a Gaussian distribution. Dry days are not corrected and will remain without precipitation even after perturbation.
Soil moisture errors are homosecdastic and not heteroscedastic. About 0.01 to 0.02 m3/m3 error seems realistic independent of measured/simulated value.

Reply: These variables which are perturbed in data assimilation are referred to rainfall, streamflow and soil moisture. Please note the standard deviation for rainfall is proportional to the magnitude of rainfall. In dry days without rainfall, the ensemble members of rainfall are equal to zero, which seems realistic to describe the rainfall field. The Gaussian distribution has been successfully used in a few studies (e.g., Moradkhani et al., 2005; Xie and Zhang, 2013). Optional distributions to describe the rainfall errors do exist, such as the uniform distribution (Clark et al., 2008), the lognormal distribution (Crow and Ryu, 2009; Chen et al., 2011) . But there is no consensus regarding which distribution is significantly better than others. The associated sentences were reworded (line 11 – 17, page 14)

It is a useful suggestion of using homoscedastic errors for soil moisture. We set the standard deviation for soil moisture as 0.03 m^3/m^3 according to studies using the SWAT model (which is also used in this study) and the Sacramento model (Crow and Ryu, 2009; Chen et al., 2011). See line 15 – 16, page 14

Review Comment 6

parameter estimations --> parameter estimates.

Reply: We corrected the misuses of “estimation”, but kept “parameter estimation” in some sentences. Thanks.

There are minor differences between “estimation” and “estimate”. An “estimation” is the process of approximately calculating or evaluating, and an “estimate” is an approximate calculation or evaluation. So an “estimate” is the result of “estimation” (http://grammarist.com/usage/).

Review Comment 7

Papers needs editing. Grammar / syntax still needs to be further improved.

Reply: We made language editing throughout the manuscript (some marked with blue). Thanks.

Review Comment 8

Conclusion section: Accumulative?

Reply: "Accumulative" was replaced by "convergent" in the revised manuscript (line 23, page 20). That sentence is to interpret that the outlet is a convergent point due to runoff routing.

Review Comment 9

"big picture" --> not very scientific.

Reply: The associated sentence was reworded: "the downstream data (especially the data from the outlet) have important roles to reflect the runoff generation for the entire basin." (line 25, page 20)

Review Comment 10

10) The parameter estimates might stabilize after relatively few assimilation steps but do they converge to their "appropriate" values. The results you get are strongly controlled by the settings of your filter. If you change some of the settings for the smoother and parameter estimation part, the filter will not converge as rapidly. moreover, is the posterior parameter uncertainty reasonable. My experience suggests that this is not the case. This is an engineering solution but violates statistical principles. A simple test can show this. Create a synthetic streamflow data set of 5 years where you use completely different parameter values for the first and second part of this data set. Then assimilate this data set using your filter. You will see that your method will not converge appropriately, and certainly cannot diagnose the suddenly varying parameter values. Why? The filter settings are set such that they promote very quick convergence of the parameter values. Once the filter has converged the parameter uncertainty is too small (and significantly underestimates the "actual" understand - the parameters will also be wrong!) - due to this small uncertainty the filter cannot travel to the new parameter values that created the second part of the time series. I consider this a serious flaw in the methodology - The results

are enforced by the user and are statistically not correct. Yes, it might improve the discharge estimates - but should one not use a statistically correct methodology?

Reply: We argue the parameter estimates converge to their "appropriate" values with reasonable uncertainties. To validate this argument, we designed a simple synthetic experiment according to the reviewer's suggestion. A synthetic streamflow data series of five years (1826 days in total) was generated based on a simulation with the SCS model (which has been coupled in the SWAT model as a runoff generation and routing modular). For the five-year simulation, different sets of parameter values were used for two successive periods (1st – 800th days, 801st – 1826th days). Specifically, the parameters have an abrupt change at the 801st time step (see the red lines in Figure 1 below). We take this setting as true values for parameters. The synthetic streamflow data were perturbed using Gaussian distribution to represent observation uncertainties, and then they were assimilated into the model. The initial realizations of parameters for data assimilation are intentionally biased to their true values.

Three cases were conducted with different smoothing factors (α = 0.99, 0.97 and 0.95). As mentioned above (the reply to comment 3), the smoothing factor generally ranges from 0.95 to 0.99, and the shrinkage factor is estimated as $\sqrt{1-\alpha^2}$ (Liu, 2000; Moradkhani et al., 2005).

Figure 1 below shows an example of the parameter estimates, i.e., the CN_2 in SWAT. For the three cases, generally, the CN_2's estimates are able to converge to its true values in the two successive periods. About 400 time steps of assimilations are required to make the estimates agree with the true. Despite the abrupt change at the

801st time step, the estimates can approach to the true value after the 1200th time steps during the second period. Moreover, the smoothing factor has a certain impact on the performance of parameter estimation. The case of α = 0.95 exhibits obvious fluctuations in the estimation process while the estimate captures the general pattern of the parameter travel. The case of α = 0.99 provides the best estimates for CN_2. In addition, the three cases maintain a certain degree of ensemble spreads which are favorable to trace the parameter travel. Obviously, the ensemble spread will shrink with the increase of α. Note it doesn't mean that large α can result in better parameter estimates in any cases. An appropriate setting for α can be obtained by a trial and error strategy.

We agree that the ensemble of parameters is prone to shrink (means too small ensemble spread/uncertainties), if the parameter is not perturbed, and consequently the estimates are difficult to trace the parameter travel. The kernel smoothing is a way to relax this problem. By adding small perturbations (equation (3)), the ensemble of parameters has a relatively broad spread to represent a reasonable uncertainties. That is why the kernel smoothing technique facilitates the parameter estimation within our data assimilation scheme (i.e., PU_EnKF).

Therefore, the PU_EnKF scheme with the kernel smoothing used in this study can achieve the correct/appropriate values of parameters with reasonable uncertainties. The kernel smoothing technique is effective to perturb the parameters. The setting for the smoothing factor has impact, to some degree, on the parameter estimation, but the performance of PU_EnKF with kernel

smoothing is robust due to acceptable convergence of parameter estimates.

We admit there are alternative methods to address state and parameter estimation (e.g., Vrugt et al., 2013; Tran et al., 2014). In future work, it is interesting to make a comparison among these methods with different hydrological models (line 16- 19, page 21).

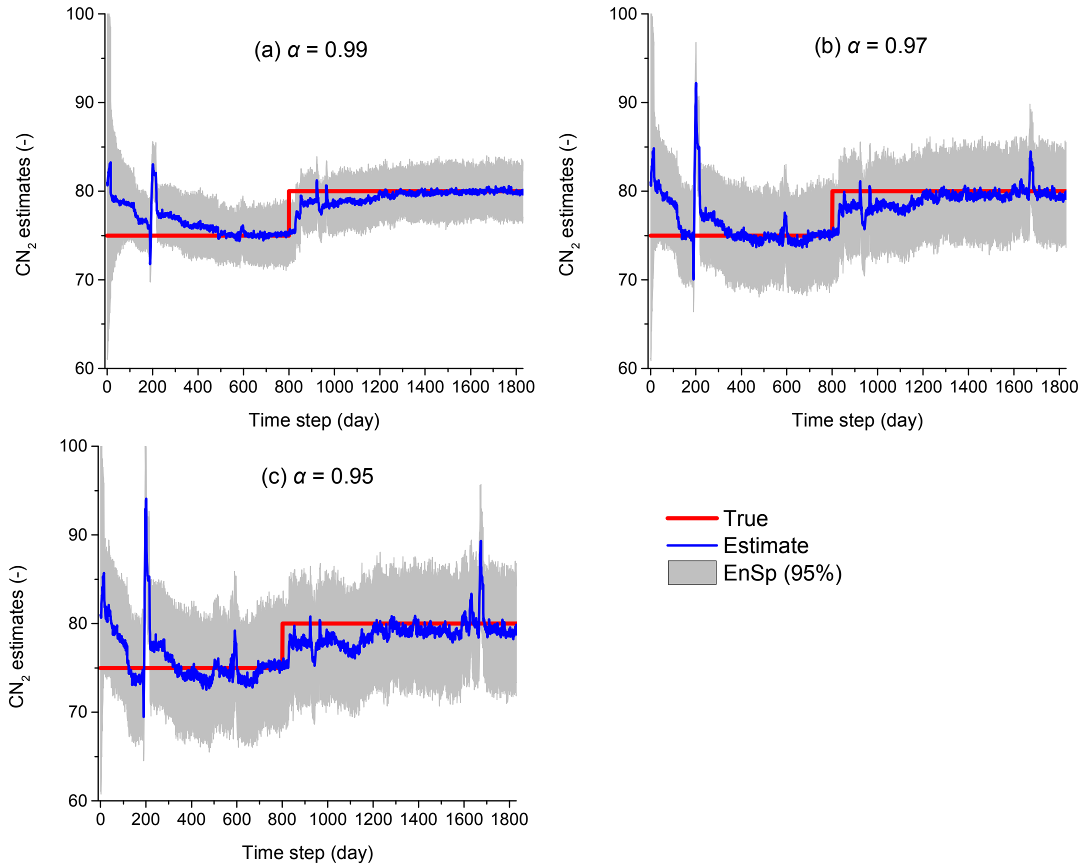

Figure 1. A synthetic case of parameter estimates with different smoothing factors (α). The blue line denotes the parameter estimate (i.e., the ensemble mean). The light gray area indicates the ensemble spread (EnSp) with 95 % confidence intervals.

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