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Simultaneous estimation of model state variables and observation and forecast biases using a two-stage hybrid Kalman filter

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Abstract

In this paper, we present a two-stage hybrid Kalman filter to estimate both observation and forecast bias in hydrologic models, in addition to state variables. The biases are estimated using the Discrete Kalman Filter, and the state variables using the Ensemble Kalman Filter. A key issue in this multi-component assimilation scheme is the exact partitioning of the difference between observation and forecasts into state, forecast bias and observation bias updates. Here, the error covariances of the forecast bias and the unbiased states are calculated as constant fractions of the biased state error covariance, and the observation bias error covariance is a function of the observation prediction error covariance. In a series of synthetic experiments, focusing on the assimilation of discharge into a rainfall-runoff model, it is shown that both static and dynamic observation and forecast biases can be successfully estimated. The results indicate a strong improvement in the estimation of the state variables and resulting discharge as opposed to the use of a bias-unaware Ensemble Kalman Filter. The results suggest that a better performance of data assimilation methods should be possible if both forecast and observation biases are taken into account.

1 Introduction

During the last decade, data assimilation has ~~become a relatively~~ [1] frequently applied ~~methodology for~~ [2] the correction of errors in hydrologic model results. These errors originate from uncertainties in meteorological forcing data, model parameters, formulation of the model physics, and initial conditions. A number of methods are available for this purpose, of which the most commonly used are Newtonian nudging (Stauffer and Seaman, 1990), the Extended Kalman Filter (Welch and Bishop, 1995), the Ensemble Kalman Filter (Evensen, 1994), variational assimilation (Rabier et al., 2000), and the Particle Filter (Gordon et al., 1993). These methods have been applied for the assimilation of various variables. Examples of these variables and studies that focus on

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their assimilation are surface soil moisture values (Crow and van den Berg, 2010), surface temperatures (Meng et al., 2009), brightness temperatures (Seuffert et al., 2004), radar backscatter values (Hoeben and Troch, 2000), snow water equivalent (De Lannoy et al., 2012), snow cover fraction (Su et al., 2010), piezometric head data (Chen and Zhang, 2006), chemical tracer data (Ng et al., 2009), and discharge values (Pauwels and De Lannoy, 2009).

In many studies, observations are used that contain both random error and significant bias (Torres et al., 2012). Furthermore, hydrologic model results do not only contain random errors, but in many cases are also prone to bias (Ashfaq et al., 2010). Typically, the above mentioned methods only function optimally when the assimilated data and the model are free of bias. In order to bypass this inconsistency, a number of studies have focused on the removal of systematic differences between the assimilated data and the model through rescaling the data to the model climatology (Reichle and Koster, 2004; Slater and Clark, 2006; De Lannoy et al., 2012). Other studies have focused on the estimation of the forecast bias in addition to the model state variabes, using the Discrete (Kalman, 1960) and the Ensemble Kalman Filter for both linear and nonlinear systems, in a wide range of applications ranging from groundwater modeling to soil moisture and temperature assimilation (Dee and Da Silva, 1998; Dee and Todling, 2000; De Lannoy et al., 2007; Drécourt et al., 2006; Bosilovich et al., 2007; Reichle et al., 2010). Dee (2005) further explains how forecast bias can be taken into account in a data assimilation system using the Kalman filter or variational assimilation as assimilation algorithm. The estimation of observation biases through data assimilation has been investigated as well. Derber and Wu (1998) present a simple observation bias estimation scheme for the assimilation of radiance data into an atmospheric model. Auligné et al. (2007) and Dee and Uppsala (2009) used a variational approach to estimate satellite data biases, while Montzka et al. (2013) used the Particle Filter for the retrieval of remotely sensed soil moisture biases. Another approach, as opposed to state updating and online bias estimation, is to update model parameters in addition

to state variables, under the assumption that all forecast bias is caused by the model parameters (Moradkhani et al., 2005).

[1]There have been two major practical approaches for forecast bias estimation with a Kalman filter: state augmentation (Kollat et al., 2011) and separate state and bias estimation (Friedland, 1969). Drécourt et al. (2006) compared both approaches using a linear groundwater model, and concluded that both methodologies outperformed the Kalman Filter without bias estimation. Two-stage state and bias estimation, referred to as Bias-Aware Kalman Filtering by Drécourt et al. (2006), is an attractive approach where the state and the forecast bias are estimated individually. Although it is clearly demonstrated that, in the presence of forecast bias, this methodology outperforms the estimation of the model state alone (Drécourt et al., 2006; De Lannoy et al., 2007), observations are assumed to be unbiased in these studies. Furthermore, we are not aware of assimilation approaches in hydrological studies that estimate both observation and forecast bias, in addition to state variables. The objective of this paper is therefore to develop a methodology, based on the Ensemble Kalman Filter (EnKF), to estimate observation and forecast biases, as well as model state variables. More specifically, the methodology of Dee and Da Silva (1998), in which two Kalman filters are applied, is expanded to include observation biases as well. The major assumption of the proposed methodology[2] ~~as opposed to state augmentation,~~ is that the observation and forecast bias errors are independent of each other and of the errors in the unbiased model state variables. This assumption needs to be made in order to enable the derivation of a separate state and bias update equation. In this paper, we will demonstrate that, despite this assumption, reasonable results can be obtained. The equations for the estimation of the biases and the state variables are derived for a linear system, after which the application for nonlinear systems in an ensemble framework is explained. The method is then applied to a very simple rainfall-runoff model, into which discharge values are assimilated, first in a well-controlled synthetic experiment, and then in a real-world example. The performance of the new methodology is then analyzed in detail,

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I find this rather inconsistent. It seems like state augmentation methods, here referenced as (Kollat, 2011), were devised after Drecourt-2006's comparison, which of course cannot be possible. Perhaps the citation [Kollat, 2011] is not appropriately chosen.

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I don't think this assumption is incompatible with state augmentation. More simply, state augmentation methods are more general than that presented here, in that they do not require independence between model and observation bias. This does not mean that this assumption could not be implemented even within a state augmentation approach.

and the possibilities for joint observation and forecast bias and model state estimation are assessed.

2 Derivation for a linear system

2.1 System Description

The equations for the simultaneous estimation of system states and both forecast and observation biases will first be derived for a linear system. The application of the analytical expressions in an ensemble framework will then be explained.

In the bias-aware Kalman filter, the state of the system is propagated from time step $k-1$ to time step k:

$$\tilde{\boldsymbol{x}}_k = \mathbf{A}_{k-1}\tilde{\boldsymbol{x}}_{k-1} + \mathbf{B}_{k-1}\boldsymbol{f}_{k-1} + \boldsymbol{w}_{k-1} \quad (1)$$

$\tilde{\boldsymbol{x}}_k$ is the biased state vector, and $\boldsymbol{f}_{k-1}$ is the vector with model inputs (for example the meteorologic input data). $\boldsymbol{w}_{k-1}$ is the model error, which is a random error term with covariance $\mathbf{Q}_{k-1}$. $\mathbf{A}_{k-1}$ and $\mathbf{B}_{k-1}$ are model matrices propagating states and forcings at time step $k-1$ to states at time k. For the remainder of the paper, variables indicated with a $[\tilde{.}]$ refer to biased variables~~, while variables without the [.] refer to unbiased variables~~. The differerence between this equation and the equation used in the derivation of the Discrete Kalman filter (Kalman, 1960) is that here biased state variables are used, ~~while the bias-free Discrete Kalman filter is derived using unbiased variables.~~

The unbiased state vector $\boldsymbol{x}_k$ is defined as:

$$\boldsymbol{x}_k = \tilde{\boldsymbol{x}}_k - \boldsymbol{b}_k^m \quad (2)$$

$\boldsymbol{b}_k^m$ is the forecast bias. The system is observed as follows:

$$\tilde{\boldsymbol{y}}_k = \mathbf{H}_k\boldsymbol{x}_k + \boldsymbol{v}_k + \boldsymbol{b}_k^{\mathrm{o}} \quad (3)$$

$\tilde{\boldsymbol{y}}_k$ is the vector with the biased observations. $\boldsymbol{v}_k$ is the ~~zero mean~~ observation error with covariance $\mathbf{R}_k$. $\mathbf{H}_k$ is the observation matrix, and $\boldsymbol{b}_k^{\mathrm{o}}$ is the observation bias. This equation differs from the equation used in the bias-free Discrete Kalman filter through the observation bias term. The unbiased observations can be calculated as:

$$\boldsymbol{y}_k = \tilde{\boldsymbol{y}}_k - \boldsymbol{b}_k^{\mathrm{o}} \quad (4)$$

~~The bias vectors are propagated as follows:~~

$$\begin{cases} \boldsymbol{b}_k^m = \boldsymbol{b}_{k-1}^m \\ \boldsymbol{b}_k^{\mathrm{o}} = \boldsymbol{b}_{k-1}^{\mathrm{o}} \end{cases} \quad (5)$$

In the derivation of the two-stage state and bias update equations, it is important to ~~stress~~ that the errors in the observation and forecast biases are assumed independent of each other and of the error in the unbiased state of the system.

2.2 Propagation of the states and biases

In a simulation framework, an estimate of the system state is used in the model. For the remainder of this paper, estimated variables are denoted with an $[\hat{.}]$. $[\hat{.}]^-$ indicates an a priori estimate (forecast, before the update), and $[\hat{.}]^+$ an a posteriori estimate (analysis, after the update). The a posteriori state estimate is propagated as follows:

$$\hat{\tilde{\boldsymbol{x}}}_k^- = \mathbf{A}_{k-1}\hat{\tilde{\boldsymbol{x}}}_{k-1}^+ + \mathbf{B}_{k-1}\boldsymbol{f}_{k-1} \quad (6)$$

The system is observed as follows:

$$\hat{\tilde{\boldsymbol{y}}}_k^- = \mathbf{H}_k\hat{\boldsymbol{x}}_k^- + \hat{\boldsymbol{b}}_k^{\mathrm{o}-} \quad (7)$$

The biase estimates are also propagated:

$$\begin{cases} \hat{\boldsymbol{b}}_k^{m-} = \hat{\boldsymbol{b}}_{k-1}^{m+} \\ \hat{\boldsymbol{b}}_k^{\mathrm{o}-} = \hat{\boldsymbol{b}}_{k-1}^{\mathrm{o}+} \end{cases} \quad (8)$$

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Several authors include an extra term at the right-hand side of Equation (1) to account for model bias. This term does not appear here, so that this looks more like an unbiased model. In this scheme, the model bias seem to be due exclusively to propagation of errors from the previous time step through the model matrix A_{k-1}. Can you comment on why this is the correct way to proceed?

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unnecessary, since implied by the previous proposition

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instead of

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zero-mean (unbiased)

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I strongly suggest removing these two equations as they may raise some confusion. Given how they are written, they indicate that both model and observation biases do not change with "k", that is, they are time-invariant (constant). This is obviously not the case, which becomes clear later from Equations (8).

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remark

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at time step k-1

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to time step k

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Note that, unlike Equation (1), Equation (6) does not directly account for model bias, which seems to propagate from the previous time step according to a model unbiased scheme (see my observation above on Eq. (1)).

2.3 Update of the states and biases

The observations are used as follows to update the states and biases:

$$\begin{cases} \hat{\boldsymbol{b}}_k^{m+} = \hat{\boldsymbol{b}}_k^{m-} + \mathbf{K}_k^m \left(\tilde{\boldsymbol{y}}_k - \hat{\boldsymbol{b}}_k^{o-} - \mathbf{H}_k \left(\hat{\tilde{\boldsymbol{x}}}_k^- - \hat{\boldsymbol{b}}_k^{m-} \right) \right) \\ \hat{\boldsymbol{b}}_k^{o+} = \hat{\boldsymbol{b}}_k^{o-} + \mathbf{K}_k^{\mathrm{o}} \left(\tilde{\boldsymbol{y}}_k - \hat{\boldsymbol{b}}_k^{o-} - \mathbf{H}_k \left(\hat{\tilde{\boldsymbol{x}}}_k^- - \hat{\boldsymbol{b}}_k^{m-} \right) \right) \\ \hat{\boldsymbol{x}}_k^+ = \hat{\tilde{\boldsymbol{x}}}_k^- - \hat{\boldsymbol{b}}_k^{m+} + \mathbf{K}_k \left(\tilde{\boldsymbol{y}}_k - \hat{\boldsymbol{b}}_k^{o+} - \mathbf{H}_k \left(\hat{\tilde{\boldsymbol{x}}}_k^- - \hat{\boldsymbol{b}}_k^{m+} \right) \right) \end{cases} \tag{9}$$

$\mathbf{K}_k^m$, $\mathbf{K}_k^{\mathrm{o}}$, and $\mathbf{K}_k$ are the Kalman gains for the forecast bias, the observation bias, and the system states, respectively. The filter thus works in two steps. First, the a priori bias and state estimates are used to update the observation and forecast bias estimates. The update is performed using the unbiased estimates: the observation bias is substracted from the observations, and the observation matrix is applied to the unbiased state vector. The a posteriori forecast bias estimate $\hat{\boldsymbol{b}}_k^{m+}$ is then used to calculate the a priori unbiased state estimate, which is defined as:

$$\hat{\boldsymbol{x}}_k^- = \hat{\tilde{\boldsymbol{x}}}_k^- - \hat{\boldsymbol{b}}_k^{m+} \tag{10}$$

This definition, in combination with the a posteriori observation bias estimates, is used to update the unbiased state estimates. It should be noted that the biased state is fed back into the model. ~~This, in~~ other words, Eq. (10) is an output equation, providing the unbiased state estimates, and is no part of the model integration. An analytical expression for the three Kalman gains is thus needed. It is relatively straightforward to prove that the last update in Eq. (9) leads to unbiased state estimates (Appendix A).

2.4 Definition of the error covariances

In order to derive an expression for the Kalman gains, a number of error covariances need to be defined. The error covariances of the unbiased states, forecast biases and

observation biases can be written as:

$$\begin{cases} \mathbf{P}_k^+ = E\left[\left(\boldsymbol{x}_k - \hat{\boldsymbol{x}}_k^+ \right) \left(\boldsymbol{x}_k - \hat{\boldsymbol{x}}_k^+ \right)^{\mathrm{T}} \right] \\ \mathbf{P}_k^{m+} = E\left[\left(\boldsymbol{b}_k^m - \hat{\boldsymbol{b}}_k^{m+} \right) \left(\boldsymbol{b}_k^m - \hat{\boldsymbol{b}}_k^{m+} \right)^{\mathrm{T}} \right] \\ \mathbf{P}_k^{\mathrm{o}+} = E\left[\left(\boldsymbol{b}_k^{\mathrm{o}} - \hat{\boldsymbol{b}}_k^{o+} \right) \left(\boldsymbol{b}_k^{\mathrm{o}} - \hat{\boldsymbol{b}}_k^{o+} \right)^{\mathrm{T}} \right] \end{cases} \tag{11}$$

Similarly, the error covariance of the biased states can be written as:

$$\tilde{\mathbf{P}}_k^+ = E\left[\left(\tilde{\boldsymbol{x}}_k - \hat{\tilde{\boldsymbol{x}}}_k^+ \right) \left(\tilde{\boldsymbol{x}}_k - \hat{\tilde{\boldsymbol{x}}}_k^+ \right)^{\mathrm{T}} \right] \tag{12}$$

2.5 The Equations for a bias-aware linear system

Appendix B provides the details of the derivation of the equations for the application of the bias-aware Kalman filter. These can be summarized as follows. The first step consists of the propagation of the system state and the biases:

$$\begin{cases} \hat{\tilde{\boldsymbol{x}}}_k^- = \mathbf{A}_{k-1} \hat{\tilde{\boldsymbol{x}}}_{k-1}^+ + \mathbf{B}_{k-1} \boldsymbol{f}_{k-1} \\ \hat{\boldsymbol{b}}_k^{m-} = \hat{\boldsymbol{b}}_{k-1}^{m+} \\ \hat{\boldsymbol{b}}_k^{\mathrm{o}-} = \hat{\boldsymbol{b}}_{k-1}^{\mathrm{o}+} \end{cases} \tag{13}$$

Equation (13) can be initialized with any appropriate prior guess, i.e. typically a spun up biased state estimate for $\hat{\tilde{\boldsymbol{x}}}_{k-1}^+$, and zero estimates for the biases. The next step ~~is~~ ~~then~~ the propagation of the error covariances:

$$\begin{cases} \mathbf{P}_k^- = \mathbf{A}_{k-1} \tilde{\mathbf{P}}_{k-1}^+ \mathbf{A}_{k-1}^{\mathrm{T}} + \mathbf{P}_k^{m+} + \mathbf{Q}_{k-1} \\ \mathbf{P}_k^{\mathrm{o}-} = \mathbf{P}_{k-1}^{\mathrm{o}+} \\ \mathbf{P}_k^{m-} = \mathbf{P}_{k-1}^{m+} \end{cases} \tag{14}$$

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I strongly suggest avoiding repeating the same Equations once again [for example: (13.a) is the same as (6); (13.b-c) are the same as (8); (19) are the same as (9.a-b); (20) is the same as (9.c)]. This makes the paper hard to follow. After reading this section I realized it includes the (procedure) sequence of equations to apply. Some equations are new, others are not. It would make more sense to merge the definition of the covariance and Kalman gain matrices in Section 2.3, and describe the update procedure in a figure illustrating, with something like a flow chart, the sequence of equations to be applied.

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I think it is worth to explain with some more detail how this would be obtained.

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consists of

Section 3.3 explains how the forecast and observation bias error covariances can be estimated in practice. The Kalman gains of the biases then need to be calculated:

$$\begin{cases} \mathbf{K}_k^{o} = \mathbf{P}_k^{o-}\left[\mathbf{H}_k\left(\tilde{\mathbf{P}}_k^{-} + \mathbf{P}_k^{m-}\right)\mathbf{H}_k^{T} + \mathbf{P}_k^{o-} + \mathbf{R}_k\right]^{-1} \\ \mathbf{K}_k^{m} = -\mathbf{P}_k^{m-}\mathbf{H}_k^{T}\left[\mathbf{H}_k\left(\tilde{\mathbf{P}}_k^{-} + \mathbf{P}_k^{m-}\right)\mathbf{H}_k^{T} + \mathbf{P}_k^{o-} + \mathbf{R}_k\right]^{-1} \end{cases} \quad (15)$$

After which the bias error covariances can be updated:

$$\begin{cases} \mathbf{P}_k^{o+} = \left[\mathbf{I} - \mathbf{K}_k^{o}\right]\mathbf{P}_k^{o-} \\ \mathbf{P}_k^{m+} = \left[\mathbf{I} + \mathbf{K}_k^{m}\mathbf{H}_k\right]\mathbf{P}_k^{m-} \end{cases} \quad (16)$$

We can then calculate the Kalman gain of the state variables:

$$\mathbf{K}_k = \mathbf{P}_k^{-}\mathbf{H}_k^{T}\left[\mathbf{H}_k\mathbf{P}_k^{-}\mathbf{H}_k^{T} + \mathbf{P}_k^{o+} + \mathbf{R}_k\right]^{-1} \quad (17)$$

Using this Kalman gain, the state error covariance can be updated:

$$\mathbf{P}_k^{+} = \left[\mathbf{I} - \mathbf{K}_k\mathbf{H}_k\right]\mathbf{P}_k^{-} \quad (18)$$

The last step is then the update of the biases and the unbiased state variables. Since in the update of the state variables the a posteriori bias estimates are needed, these need to be updated first:

$$\begin{cases} \hat{\boldsymbol{b}}_k^{m+} = \hat{\boldsymbol{b}}_k^{m-} + \mathbf{K}_k^{m}\left(\tilde{\boldsymbol{y}}_k - \hat{\boldsymbol{b}}_k^{o-} - \mathbf{H}_k\left(\hat{\tilde{\boldsymbol{x}}}_k^{-} - \hat{\boldsymbol{b}}_k^{m-}\right)\right) \\ \hat{\boldsymbol{b}}_k^{o+} = \hat{\boldsymbol{b}}_k^{o-} + \mathbf{K}_k^{o}\left(\tilde{\boldsymbol{y}}_k - \hat{\boldsymbol{b}}_k^{o-} - \mathbf{H}_k\left(\hat{\tilde{\boldsymbol{x}}}_k^{-} - \hat{\boldsymbol{b}}_k^{m-}\right)\right) \end{cases} \quad (19)$$

Finally, we can then update the unbiased state estimate:

$$\hat{\boldsymbol{x}}_k^{+} = \hat{\tilde{\boldsymbol{x}}}_k^{-} - \hat{\boldsymbol{b}}_k^{m+} + \mathbf{K}_k\left(\tilde{\boldsymbol{y}}_k - \hat{\boldsymbol{b}}_k^{o+} - \mathbf{H}_k\left(\hat{\tilde{\boldsymbol{x}}}_k^{-} - \hat{\boldsymbol{b}}_k^{m+}\right)\right) \quad (20)$$

2.6 Interpretation of the expressions for the Kalman gains

Equations (15) and (17) list the expressions for the three Kalman gains. These expressions can be compared to the expression for the Kalman gain for a linear, bias-unaware (or unbiased) system:

$$\mathbf{K}_k^{l} = \mathbf{P}_k^{-}\mathbf{H}_k^{T}\left[\mathbf{H}_k\mathbf{P}_k^{-}\mathbf{H}_k^{T} + \mathbf{R}_k\right]^{-1} \quad (21)$$

In the above derived expressions, firstly the observation bias error covariance appears. For the bias estimation, the a priori bias error covariances are used, while for the state update Kalman gain the a posteriori error covariance is needed. This is a logical consequence of Eq. (9), where the a priori observation bias is substracted from the biased observations in the innovations, while the a posteriori bias estimation is used in the state update.

Further, for the bias Kalman gains (Eq. 15), both $\mathbf{H}_k\mathbf{P}_k^{m-}\mathbf{H}_k^{T}$ and $\mathbf{H}_k\tilde{\mathbf{P}}_k^{-}\mathbf{H}_k^{T}$ appear in the denominator, while for the state Kalman gain, the denominator contains $\mathbf{H}_k\mathbf{P}_k^{-}\mathbf{H}_k^{T}$. This can again be explained by the update equations (Eq. 9). For the bias updates, $\mathbf{H}_k\left(\hat{\tilde{\boldsymbol{x}}}_k^{-} - \hat{\boldsymbol{b}}_k^{m-}\right)$ is substracted from the observations. $\hat{\tilde{\boldsymbol{x}}}_k^{-} - \hat{\boldsymbol{b}}_k^{m-}$ is defined as the a priori estimate of the unbiased state, with an error covariance matrix equal to $\tilde{\mathbf{P}}_k^{-}$-$\mathbf{P}_k^{m-}$. Both these error covariances are used in the Kalman gain. For the system state update, $\hat{\boldsymbol{x}}_k^{-}$ appears in the innovation, and the unbiased error covariance $\mathbf{P}_k^{-}$ is thus used (Eq. 17).

As a summary, the Kalman gain takes into account the uncertainty of all the terms in the update equation, which explains the different terms in the denominator for the three Kalman gain expressions.

A further difference between ~~on the one hand~~ the Kalman gains for the system state and forecast bias, and ~~on the other hand~~ the Kalman gain for the observation bias, is that the first factor in the Kalman gain expression for the system state and forecast bias is multiplied by $\mathbf{H}_k^{T}$, while for the observation bias Kalman gain it is not. This can be explained by the remapping of the system state and forecast bias to the observation

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(Equation 15.b)

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Please explain what the "innovations" are. A reader that is not expert on data assimilation will not know what they are otherwise.

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(Equation 17)

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I found this difference almost trivial. I suggest removing this paragraph.

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space, which is necessary for the system state and forecast bias, while for the observation bias it is not.

A final remark is the minus that appears in the expression for the forecast bias Kalman gain. This can be explained by the definition of the forecast bias (Eq. 2) and the observation bias (Eq. 4). A positive forecast bias means that the biased state is larger than the unbiased state. A similar remark can be made regarding the observation bias. Assume a model with a positive forecast and observation ~~bias~~. Further, assume a positive observation system (in other words, all nonzero entries in $\mathbf{H}_k$ are positive). This means that an increase in the state variables will lead to an increase in the observation. Assume also that the unbiased observation predictions are smaller than the actual unbiased observations (meaning that the expression between brackets in Eq. 9 is positive). This may imply that either the biased system state is underestimated, or the forecast bias is overestimated, or the observation bias is underestimated, or a combination of these possibilities. The possible overestimation of the forecast bias explains the minus in the expression for the forecast bias Kalman gain.

2.7 Interpretation of the method

The objective of this method is to separate the mismatch between the observations and the model results into forecast and observation bias, and random model and observation error. This is an additional difficulty as compared to the bias-unaware KF, where this mismatch is separated into random model and observation error. The Kalman Gain (Eq. 21) can be interpreted as the fraction of this mismatch that is assigned to the model noise, and maps this mismatch from observation space onto state space through the observation operator $\mathbf{H}_k$. A similar reasoning can be made for the bias-aware KF. The Kalman Gains $\mathbf{K}_k^m$, $\mathbf{K}_k^o$ (Eq. 15), and $\mathbf{K}_k$ (Eq. 17) indicate the fraction of the mismatch that can be attributed to the forecast bias, the observation bias, and the random forecast error, respectively, and for the forecast bias and state estimates remap the difference between the unbiased observations and the unbiased simulations thereof to state space.

Equation (14) also shows that the propagation of the prior unbiased state error covariance contains an extra term as compared to the propagation for a bias-unaware (or unbiased) linear system:

$$\mathbf{P}_k^- = \mathbf{A}_{k-1}\mathbf{P}_{k-1}^+\mathbf{A}_{k-1}^\mathrm{T} + \mathbf{Q}_{k-1} \tag{22}$$

More specifically, the a posteriori forecast bias error covariance needs to be added to the forecast error covariance (the term $\mathbf{P}_k^{m+}$). This can be explained by the update equations. Essentially, Eq. (1) shows that in the system the biased state vector is propagated. The propagation of the biased state error covariace thus appears in Eq. (14). However, in the calculation of the unbiased state, the forecast bias is substracted. This implies that the unbiased state error will consist of the error in the biased state and the forecast bias, which explains the extra term in Eq. (14). The definition of the unbiased state forecast (or prior state) in Eq. (10) explains why the posterior estimate of the forecast bias error covariance is used in Eq. (14).

3 ~~Application in ensemble framework~~

3.1 General approach

The equations in Sect. 2.5 can ~~easily be~~ modified for an application in a nonlinear system. In this respect, a distinction must be made between the system model and the bias models. In Eq. (5) persistent (and thus linear) bias models are used, while the system matrix $\mathbf{A}_{k-1}$ ~~will be~~ replaced by a nonlinear model. One logical way to apply the bias-aware Kalman filter is thus to have a mix between an EnKF for the system state, and a Discrete KF for the biases.

The use of a persistent bias model is by itself an argument for separate bias-estimation with a Discrete KF. Because of the persistent nature of the bias model, an initial spread in the ensemble of biases would remain unaltered during forecast periods and decrease at each analysis step. The latter would cause filter divergence, unless

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Would the method presented here be prone to finding model bias in a case where the model was in fact unbiased? Please respond to this question where you see most appropriate in the manuscript.

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I suggest rewording this paragraph by stating first that the minus sign in Equation (15.a) is a direct result of the derivation shown in Appendix B. Then the practical explanation provided here can be given. Otherwise it makes the reader think that the minus sign is just an artifact for making model results match.

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biases

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Given the title of Section 2, I would change this to "Application to non-linear systems"

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be easily

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is

Number: 9 Author: Subject: Highlight Date: 6/17/13 1:32:55 PM some artificial inflation would be applied, which is likely to lead to inconsistencies between the state and bias estimates. Here, we will leverage off the ensemble state error covariance to approximate the bias error covariance estimate for the Discrete KF.

It should be noted that the mixed approach (an EnKF for the system states and a Discrete KF for the biases) has been applied in several studies focusing on bias estimation, such as for example De Lannoy et al. (2007). This approach is thus extended here, for the inclusion of observation biases.

3.2 Two-stage state and bias estimation versus state augmentation

A two-stage filter has a number of advantages over state augmentation. Firstly, the dimensions of the state vector do not increase. For a small number of state variables this may not be important, but for large systems this can be a considerable advantage. The calculation of the forecast error covariance requires $n_\mathrm{s}^2 \cdot n_\mathrm{e}$ calculations (with n_s the number of state variables and n_e the number of ensemble members). If the biases are added to the state vector, the calculation of $\mathbf{P}_k^-$ would require $(2n_\mathrm{s} + n_\mathrm{o})^2 \cdot n_\mathrm{e}$ calculations (with n_o the number of observations). The increase in the required number of calculations thus evolves approximately quadratically with the number of state variables, which can be a significant drawback for large systems. It should be noted that in the application of the EnKF the forecast error covariance does not need to be calculated explicitly. However, the cross-covariance between the system states and the observation simulations needs to be calculated, and a similar reasoning can be made. Another advantage is that, if a model already contains a bias-unaware EnKF, the bias-aware filter equations show that minimal code modification is needed to include the bias estimates.

The separate bias and state estimation is possible through the assumption of uncorrelated state and bias errors. State augmentation could take these correlations into account, but is computationally more expensive through the calculation of the cross-covariance between the system states and the observation simulations.

3.3 Estimation of the error covariances

Equations (15) and (17) show that a number of error covariances are needed: $\tilde{\mathbf{P}}_k^-$, $\mathbf{P}_k^-$, $\mathbf{P}_k^{m-}$, $\mathbf{P}_k^{\mathrm{o}-}$, and $\mathbf{P}_k^{\mathrm{o}+}$. These error covariances determine the partitioning of the difference between the observations and forecasts into the different error and bias components. However, it is not straightforward to optimally estimate each of these error covariances. Here, we describe some assumptions made for this paper. The biased state error covariance is given by:

$$\tilde{\mathbf{P}}_k^- = \mathbf{P}_k^- - \mathbf{P}_k^{m-} \tag{23}$$

In order to estimate the forecast bias error covariance, one thus needs to know the unbiased and the biased state error covariances. In this paper, we assume that the unbiased state error covariance is a specified fraction of the biased state error covariance. This is an approach that is used in many papers focusing on the estimation of biases through data assimilation, including Dee and Da Silva (1998), Drécourt et al. (2006), and De Lannoy et al. (2007). Calculating the biased state error covariance using the ensemble results, we can thus write:

$$\begin{cases} \mathbf{P}_k^- = \gamma \tilde{\mathbf{P}}_k^- \\ \mathbf{P}_k^{m-} = (1-\gamma)\tilde{\mathbf{P}}_k^- \end{cases} \tag{24}$$

γ is a filter parameter, between zero and one, which can be obtained through calibration. A value of zero indicates that the entire model error is assumed to be caused by bias, while a value of one indicates that noise is the only cause of errors in the model results.

The observation bias error covariances can be estimated under the assumption that a more uncertain observation prediction is accompanied by a more uncertain observation bias. For this reason, we estimate $\mathbf{P}_k^{\mathrm{o}-}$ as a function of the error covariance of the observation predictions:

$$\mathbf{P}_k^{\mathrm{o}-} = \kappa \mathbf{H}_k \tilde{\mathbf{P}}_k^- \mathbf{H}_k^\mathrm{T} \tag{25}$$

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I found this part very unclear. I think some more detailed explanations are necessary. I have a vague impression that these comments refer to findings of previous works. If this is the case, these works should be explicitly cited.

Number: 2 Author: Subject: Inserted Text Date: 6/17/13 11:46:04 AM

(De Lannoy et al., 2007).

Number: 3 Author: Subject: Line Date: 6/17/13 1:33:14 PM

Question: If augmentation was applied would this still constitute a two-stage DKF-EnKF process?

Number: 4 Author: Subject: Inserted Text Date: 6/17/13 1:33:21 PM

(reference?)

Number: 5 Author: Subject: Highlight Date: 6/17/13 11:53:03 AM

I find this as a clear advantage of the data assimilation framework presented in this manuscript, which would make it attractive for the application to other cases involving more complex distributed models. I would make sure this advantage is adequately remarked in the conclusions.

Number: 6 Author: Subject: Highlight Date: 6/17/13 11:58:59 AM

Are you saying, in other words, that the DKF portion of the scheme, would not be applicable in this case?
Would the state augmentation require using an ensemble-based approach even for the two (model and measurement) biases?

Number: 7 Author: Subject: Highlight Date: 6/17/13 8:15:58 PM

This a key assumption for the formulation and the application of the two-stage KF process presented here. Needless to say, the assumption may seem very weak if a strong physical basis is not provided.
I am not saying the assumption is wrong or right, but one needs to understand clearly where it comes from, when it is valid and when it is not. I strongly suggest the Authors to address it more thoroughly in the manuscript. In practical terms, when is this assumption realistic and when is it not? If a (parameter) spatially distributed model was applied instead of the model presented in Section 6, would this assumption still make sense?

Number: 8 Author: Subject: Cross-Out Date: 6/17/13 12:48:00 PM

κ is a filter parameter and can be estimated through calibration. Determining a typical value for this parameter is not straightforward, as it will depend on the magnitude of the different state variables and observations.

γ and κ can thus be tuned in order to optimize the filter performance. If the biases are correctly estimated, the innovations in the update equation (Eq. 20) should consist of white noise, since the bias is removed from both the observations and the simulations. This means that the autocorrelation length of these zero-mean innovations should be zero. Both parameters can thus be tuned in order to reach this zero value. An example of this filter parameter tuning is demonstrated in Sect. 7.2.

3.4 Summary

As a summary, the bias-aware EnKF can be applied as follows. First, the states and biases are propagated from time step $k-1$ to time step k:

$$\begin{cases} \hat{\tilde{\boldsymbol{x}}}_k^{i-} = f_{k,k-1}\left(\hat{\tilde{\boldsymbol{x}}}_{k-1}^{i+}, \boldsymbol{w}_{k-1}^{i}\right) \\ \hat{\boldsymbol{b}}_k^{m-} = \hat{\boldsymbol{b}}_{k-1}^{m+} \\ \hat{\boldsymbol{b}}_k^{o-} = \hat{\boldsymbol{b}}_{k-1}^{o+} \end{cases} \tag{26}$$

$f_{k,k-1}(.)$ is a nonlinear operator representing the model in state-space, including the model parameters and the meteorological forcings. i is the ensemble member number, and $\boldsymbol{w}_{k-1}^{i}$ is a realization of the model error, which can be obtained by a perturbation of the model parameters, state variables, and/or meteorological forcings.

The next step is then the calculation of $\tilde{\mathbf{P}}_k^-$ using the ensemble results:

$$\begin{cases} \tilde{\mathbf{P}}_k^- = \frac{1}{N-1}\mathbf{D}_k\mathbf{D}_k^{\mathrm{T}} \\ \mathbf{D}_k = \left[\hat{\tilde{\boldsymbol{x}}}_k^{1-} - \hat{\tilde{\boldsymbol{x}}}_k^{-}, \ \ldots, \ \hat{\tilde{\boldsymbol{x}}}_k^{N-} - \hat{\tilde{\boldsymbol{x}}}_k^{-}\right] \\ \hat{\tilde{\boldsymbol{x}}}_k^{-} = \frac{1}{N}\sum_{i=1}^{N}\hat{\tilde{\boldsymbol{x}}}_k^{i-} \end{cases} \tag{27}$$

N is the number of ensemble members. $\mathbf{P}_k^-$ and $\mathbf{P}_k^{m-}$ are then calculated using Eq. (24), and $\mathbf{P}_k^{o-}$ is calculated using Eq. (25). The three Kalman gains are then calculated using Eqs. (15) and (17). Following Reichle et al. (2002), $\mathbf{P}_k^-\mathbf{H}_k^{\mathrm{T}}$ can be calculated as the covariance between the unbiased state and the measurement predictions, and $\mathbf{H}_k\mathbf{P}_k^-\mathbf{H}_k^{\mathrm{T}}$ as the covariance of the unbiased measurement predictions. Analoguously, $\tilde{\mathbf{P}}_k^-\mathbf{H}_k^{\mathrm{T}}$ and $\mathbf{H}_k\tilde{\mathbf{P}}_k^-\mathbf{H}_k^{\mathrm{T}}$ can be calculated using the biased model results. This implies that $\mathbf{P}_k^-$ and $\tilde{\mathbf{P}}_k^-$ do not need to be calculated explicitly.

Before calculating the state Kalman gain, $\mathbf{P}_k^{o-}$ needs to be updated to $\mathbf{P}_k^{o+}$, since this is needed in the expression (Eq. 17). This is performed by:

$$\mathbf{P}_k^{o+} = \mathbf{P}_k^{o-}\left[\mathbf{I} - \mathbf{K}_k^{o}\right] \tag{28}$$

Using the calculated Kalman gains and observation bias error covariance, the state variables and the biases can then be updated:

$$\begin{cases} \hat{\boldsymbol{b}}_k^{m+} = \hat{\boldsymbol{b}}_k^{m-} + \mathbf{K}_k^{m}\left(\tilde{\boldsymbol{y}}_k - \hat{\boldsymbol{b}}_k^{o-} - \overline{h_k\left(\hat{\tilde{\boldsymbol{x}}}_k^{i-} - \hat{\boldsymbol{b}}_k^{m-}\right)_{i=1,\ldots,N}}\right) \\ \hat{\boldsymbol{b}}_k^{o+} = \hat{\boldsymbol{b}}_k^{o-} + \mathbf{K}_k^{o}\left(\tilde{\boldsymbol{y}}_k - \hat{\boldsymbol{b}}_k^{o-} - \overline{h_k\left(\hat{\tilde{\boldsymbol{x}}}_k^{i-} - \hat{\boldsymbol{b}}_k^{m-}\right)_{i=1,\ldots,N}}\right) \\ \hat{\boldsymbol{x}}_k^{i+} = \hat{\tilde{\boldsymbol{x}}}_k^{i-} - \hat{\boldsymbol{b}}_k^{m+} + \mathbf{K}_k\left(\tilde{\boldsymbol{y}}_k - \hat{\boldsymbol{b}}_k^{o+} - h_k\left(\hat{\tilde{\boldsymbol{x}}}_k^{i-} - \hat{\boldsymbol{b}}_k^{m+}\right) + \boldsymbol{v}_k^{i}\right) \end{cases} \tag{29}$$

$h_k(.)$ is a nonlinear function, relating the state variables to the observations. Note that the two bias update equations are deterministic, while the third state update equation is performed for each individual ensemble member. i is the ensemble member, and $\overline{h_k\left(\hat{\tilde{\boldsymbol{x}}}_k^{i-} - \hat{\boldsymbol{b}}_k^{m-}\right)_{i=1,\ldots,N}}$ indicates the average simulated observations, calculated across the ensemble. $\boldsymbol{v}_k^{i}$ is a random realization of the observation error, and is needed in order to ensure a sufficient ensemble spread (Burgers et al., 1998).

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Number: 1 Author: Subject: Cross-Out Date: 6/17/13 12:48:14 PM

Number: 2 Author: Subject: Sticky Note Date: 6/17/13 12:47:12 PM

Number: 3 Author: Subject: Highlight Date: 6/17/13 10:00:04 PM

How are these calibrations performed? While I understand that a precise answer cannot be given at this point since the model has not yet been introduced, it would be instructive to provide general notions as to how and with respect to what this calibration is achieved.
My (vague) understanding is that the idea behind this calibration is to force the ensemble of unbiased states to be "stationary" (with zero mean deviation) around the (unknown) true state.
Is that correct? Is so please provide a similar observation in the narrative.

Number: 4 Author: Subject: Inserted Text Date: 6/17/13 12:48:45 PM

Both coefficients

Number: 5 Author: Subject: Inserted Text Date: 6/17/13 12:50:45 PM

calibrated

Number: 6 Author: Subject: Highlight Date: 6/17/13 1:14:12 PM

As for Section 2.5, I strongly suggest avoiding repeating the same Equations once again [for example: (26.b-c) are the same as (8)].

Number: 7 Author: Subject: Highlight Date: 6/17/13 1:11:37 PM

Note that Equation (26.a) does not directly account for model bias, which seems to propagate from the previous time step according to a model unbiased scheme (see my observation above on Equation 1).

4 Evaluation of the methodology

The derived equations are tested through a synthetic study. A very simple rainfall-runoff model is first calibrated for the Zwalm catchment in Belgium. The obtained parameters are then used to generate discharge and storage values. The synthetically true storages are obtained by adding a predefined bias to the modeled storage values (which is consistent with Eq. 2). The synthetic discharge observations are then obtained by adding a predefined observation bias to the discharge, obtained with these biased storages. Furthermore, a random-error term with a predefined standard deviation is added to the synthetic discharge observations as well. This is consistent with Eq. (3). The synthetic observations are then assimilated into the model, and the retrieved storages and discharges can then be compared to the synthetic truth in order to evaluate the performance of the data assimilation algorithm.

In order to thoroughly evaluate the performance of the filter, three experiments are performed. Table 1 shows an overview of these experiments. The first experiment considers only observation bias and noise, and no forecast bias. In order to generate the synthetic truth, no bias is added to the storages, and a bias of 0.5 $m^3 s^{-1}$ and a random error with a standard deviation of 0.1 $m^3 s^{-1}$ are added to the synthetically true discharge. These synthetic observations are then assimilated into the model with an assimilation interval of 7 days. All observations could have been assimilated as well (thus an update at every time step), but this would not as clearly demonstrate the impact of the bias estimation.

The second experiment considers observation bias and noise as well as forecast bias. Again, a bias of 0.5 $m^3 s^{-1}$ and a random error with a standard deviation of 0.1 $m^3 s^{-1}$ are added to the synthetically true discharge. However, in order to generate the synthetic truth, bias is added to the storages. Forecast bias is generated this way, in a manner consistent with the filter theory, and ~~it can then be assessed~~ to what extent the bias-aware EnKF will correctly estimate the true storage and discharge values. The value of the bias added to the storages is obtained by examining the standard

deviation in the modeled storages, obtained using the calibrated model parameters. The bias was then assumed to be 10 % of this standard deviation. This resulted in a bias of 20 mm, 0.4 mm, and 0.2 mm for the surface, slow reservoir, and fast reservoir storages, respectively (see Sect. 6).

The third experiment considers only observation noise and forecast bias. A random error with a standard deviation of 0.1 $m^3 s^{-1}$ is added to the synthetically true discharge, which is again obtained by adding a predefined bias to the storage values.

In order to investigate the possibility to estimate a temporally varying observation and forecast bias, the three experiments are repeated, but with a sinus wave added to the mean biases. The period of this wave is equal to one year and the amplitude equal to 0.25 $m^3 s^{-1}$ for the observation bias, and 10 mm, 0.2 mm, and 0.1 mm for the surface, slow reservoir, and fast reservoir storages, respectively.

5 Site and data description

The study is performed in the Zwalm catchment in Belgium. Troch et al. (1993) provide a complete description of this test site, only a very short overview ~~will be~~ given here. The total drainage area of the catchment is 114.3 km^2 and the total length of the perennial channels is 177 km. The maximum elevation difference is 150 m. The average annual temperature is 10 °C, with January the coldest month (mean temperature 3 °C) and July the warmest month (mean temperature 18 °C). The average annual rainfall is 775 mm and is distributed evenly throughout the year. The annual actual evapotranspiration is approximately 450 mm.

Meteorological forcing data with a ~~daily resolution (the model~~ time step) from 1994 through 2002 were used in this study. The precipitation and all the variables needed to calculate the potential evapotranspiration using the Penman–Monteith equation were measured by the meteorological station in Kruishoutem. Discharge was measured continuously at the catchment outlet in Nederzwalm.

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Number: 1 Author: Subject: Sticky Note Date: 6/17/13 1:19:35 PM

I would suggest changing "storages" to "storage values" throughout the paper.

Number: 2 Author: Subject: Highlight Date: 6/17/13 10:20:45 PM

I think most of the information given in this section, in particular the description of the simulated scenarios, and the hypothesized observation and model biases should be given after the site and the model have been described. With some due arrangements Section 4 should be moved after Sections 5 and 6. The reader would not be able to understand what the prescribed model bias and observation bias are before the model and the observed data are presented.

Number: 3 Author: Subject: Highlight Date: 6/17/13 10:21:41 PM

I am not sure on why this would not. However, since this information is probably not relevant as given here, I would suggest removing it.

Number: 4 Author: Subject: Inserted Text Date: 6/17/13 1:19:00 PM

one can assess

Number: 5 Author: Subject: Inserted Text Date: 6/17/13 1:34:39 PM

is

Number: 6 Author: Subject: Cross-Out Date: 6/17/13 1:34:21 PM

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one-day

6 Model description

The Hydrologiska Byråns Vattenbalansavdelning (HBV) model, of which Fig. 1 shows a schematic, was originally developed by Linström et al. (1997). In this paper, the version of Matgen et al. (2006) is applied. The model uses observed precipitation ($R_{tot}(t)$) and potential evapotranspiration (ETP(t)) as input, both in m s^{-1}. t is the time in seconds. The catchment is divided into a soil reservoir, a fast reservoir, and a slow reservoir. There are thus three state variables: the amount of water in the soil reservoir ($S(t)$, m), the slow reservoir ($S_1(t)$, m), and the fast reservoir ($S_2(t)$, m).

A number of fluxes are calculated, which depend on the state variables of the system. The actual evapotranspiration ETR(t) (m^3 s^{-1}) is first determined:

$$\mathrm{ETR}(t) = \frac{1}{\lambda}\frac{S(t)}{S_{\max}}\mathrm{ETP}(t) \tag{30}$$

λ is a dimensionless parameter, and $S_{\max}$ is the storage capacity of the soil reservoir (m). The infiltration $R_{in}(t)$ (m s^{-1}) is calculated as follows:

$$R_{in}(t) = \left(1 - \frac{S(t)}{S_{\max}}\right)^{b} R_{tot}(t) \tag{31}$$

b is a dimensionless parameter. After this, the effective precipitation $R_{eff}(t)$ (m s^{-1}) is determined:

$$R_{eff}(t) = R_{tot}(t) - R_{in}(t) \tag{32}$$

The calculation of the percolation $D(t)$ (m s^{-1}) is then performed:

$$D(t) = \mathrm{Pe}\left(1 - e^{-\beta\frac{S(t)}{S_{\max}}}\right) \tag{33}$$

Pe is a percolation parameter (m s^{-1}), and β a dimensionless parameter. After this, the storage in the soil reservoir at the end of the time step can be calculated as follows:

$$S(t+\Delta t) = S(t) + (R_{in}(t) - \mathrm{ETR}(t) - \mathrm{Perc}(t))\,\Delta t \tag{34}$$

Δt is the time step in seconds. $S(t+\Delta t)$ is always positive after model calibration.

The input in the fast reservoir $R_2(t)$ (m s^{-1}) is then:

$$R_2(t) = \alpha\frac{S(t)}{S_{\max}}R_{eff} \tag{35}$$

α is a dimensionless parameter. The outflow from this reservoir $Q_2(t)$ (m^3 s^{-1}) is then determined:

$$Q_2(t) = \kappa_2\left(\frac{S_2(t)}{S_{2,\max}}\right) \tag{36}$$

$S_{2,\max}$ is the storage capacity of the fast reservoir (m), and κ_2 (m^3 s^{-1}) and γ (–) are model parameters. After this, the storage in the fast reservoir at the end of the time step can be calculated as:

$$S_2(t+\Delta t) = S_2(t) + (R_2(t) - Q_2(t))\,\Delta t \tag{37}$$

The input in the slow reservoir $R_1(t)$ (m s^{-1}) is then computed:

$$R_1(t) = R_{eff}(t) - R_2(t) \tag{38}$$

The outflow from this reservoir $Q_1(t)$ (m^3 s^{-1}) can be calculated as:

$$Q_1(t) = \kappa_1 S_1(t) \tag{39}$$

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R_{eff}(t)

Number: 2 Author: Subject: Highlight Date: 6/17/13 10:22:47 PM

Please use another symbol here. \gamma is already used in Equation (24).

κ_1 is a model parameter ($m^2 s^{-1}$). Finally, the storage in the slow reservoir at the end of the time step is calculated:

$$S_1(t+\Delta t) = S_1(t) + (R_1(t) - Q_1(t) + \mathrm{Perc}(t))\,\Delta t \quad (40)$$

The total discharge $q(t)$ is simply the sum of $Q_1(t)$ and $Q_2(t)$. A triangular unit hydrograph is used for runoff routing. Since in this paper daily time steps are used, and the concentration time of the catchment is only 14 h (Ferket et al., 2008), no routing needs to be performed for this study.

As a summary, the model contains ten time-invariant parameters (λ, S_{max}, b, α, P_e, β, γ, $S_{2,max}$, κ_2, and κ_1), and three state variables per time step (the storages $S(t)$, $S_1(t)$, and $S_2(t)$).

The model was calibrated using Particle Swarm Optimization (Kennedy and Eberhart, 1995), using the data from 1994 through 1997. Table 2 lists the obtained parameter values, and Fig. 2 shows the comparison of the modeled to the observed discharge for the entire simulation period. Based on these results, the rainfall-runoff dynamics of the model are deemed to be sufficiently accurate to be used in a data assimilation study.

7 Results

7.1 Ensemble generation

The experiments are applied with an ensemble of [1]2 members. The ensemble is generated by adding a Gaussianly distributed random number with zero mean to [2]ach parameter value. The standard deviation of this random number is set to a fraction of the original parameter value. It was ensured that the parameter values did not exceed physical limits. At each time step, a random error is added to the observed precipitation and potential evapotranspiration. Again, the standard deviation of the random error is set to a fraction of the original observed value. The fractions to calculate the standard

deviations are for each experiment calibrated to ensure an adequate ensemble spread following De Lannoy et al. (2006).

7.2 Filter parameter estimation

Another issue in the application of the bias-aware EnKF is the estimation of the parameters γ (used in Eq. 24 to estimate $\mathbf{P}_k^-$ and $\mathbf{P}_k^{m-}$) and κ (used in Eq. 25). The objective of the determination of these parameters is to obtain stable bias estimates, meaning that the estimates do not continue to decrease or increase as the simulation proceeds. γ is clearly a value between zero and one, while an indicative value for κ is more difficult to determine. It has been found that a too low value for κ leads to observation bias estimates that diverge from the true value during the simulation. Figure 3 shows this for experiment two [3] constant observation bias). The observation bias and the biases for S and S_1 evolve to clearly unrealistic values. A value of 100 for κ can be seen to lead to stable observation bias estimates. The results of the filter have been found to be less sensitive to the value of γ. A value of 0.1 for this parameter has been found to lead to stable estimates of the forecast bias. [4]s explained in Sect. 3.3, the autocorrelation length of the innovations in Eq. (20) should be zero with a zero mean. Figure 4 shows the ensemble average of the autocorrelation functions for each ensemble member for the case of sinusoidal observation and forecast biases. Clearly, for all lags larger than 0, the autocorrelations approach zero, which indicates that γ has been adequately estimated.

7.3 State and bias estimation for a constant observation and forecast bias

Figure 5 shows the estimated storages for each of the experiments described above, using a constant observation bias. Figure 6 shows the analysis of the modeled discharges, and the evolution of the estimated observation bias. For each of the three experiments, the estimated unbiased storages and discharges are compared to the

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Number: 1 Author: Subject: Highlight Date: 6/17/13 10:24:27 PM

As in any Monte Carlo simulation exercise, it is appropariate to provide detailed information on how the ensemble size is selected, especially if such a low value is used.

Number: 2 Author: Subject: Highlight Date: 6/17/13 1:40:16 PM

Please explain if this refers to each of the 10 parameters mentioned above.

Number: 3 Author: Subject: Inserted Text Date: 6/17/13 1:40:35 PM

2

Number: 4 Author: Subject: Highlight Date: 6/17/13 1:46:44 PM

I found this part very difficult to follow. I understand this is related to the process followed to calibrated \gamma and k, which was somehow introduced in Section 3.3. Please make a strong effort to clarify.

storages obtained using a bias-unaware EnKF in which only states are estimated and biases are not taken into account.

Examining the results of experiment 1 (only observation bias), the advantage of the bias estimation is evident. The bias-unaware EnKF leads to relatively large errors in the storages, which practically disappear when bias is taken into account. Figure 6 shows that taking into account the observation bias also leads to an almost perfect estimate of the discharge. The observation bias shows fluctuations around the mean value, but the true value of $0.5\,\mathrm{m^3\,s^{-1}}$ is retrieved ~~relatively accurately~~. [1]

Similar conclusions, but to a lesser extent, can be drawn for the results of experiment 2 (both observation and forecast bias). Figure 5 shows that the estimation for the three storages is better for the bias-aware EnKF as compared to the bias-unaware EnKF. For S_1 and S_2 an almost perfect estimate is obtained, while for S the bias is reduced but not eliminated. However, as S does not directly influence the discharge (see the equations in Sect. 6), this should not lead to errors in the discharge estimation. Figure 6 shows that indeed the discharge is almost perfectly estimated, and that the estimated bias fluctuates around the correct value.

Regarding experiment 3 (only forecast bias), the results from the bias-aware EnKF are better than for the bias-unaware EnKF. Figure 5 shows that for S the improvement is marginal, but for S_1 and S_2 a reduction in the RMSE can be observed, while the bias in the estimates is almost unaltered. Figure 6 shows that the discharge is almost perfectly estimated, and that the estimation of the observation bias again fluctuates around the correct value. In experiment 2 and 3, S remains biased due to an observability issue: the observed (assimilated) discharge is not directly related to S, and hence this information cannot be efficiently used to update the bias estimate.

Further examination of Figs. 5 and 6 shows that the estimated storages and discharges obtained using the bias-aware EnKF are almost identical for experiment 2 and experiment 3. This can be explained by the relatively accurate estimation of the observation bias. Since the bias-unaware EnKF does not take this into account, the results

for experiment 3 (where no observation bias is present) are significantly better than the results for experiment 2 for the bias-unaware EnKF.

Table 3 shows the relative RMSE increase for both the bias-aware and the bias-unaware EnKF. This relative increase is defined as:

$$\mathrm{RI} = 100\frac{\mathrm{RMSE_a} - \mathrm{RMSE_b}}{\mathrm{RMSE_b}} \tag{41}$$

RI is the relative increase (%), $\mathrm{RMSE_a}$ the RMSE of the assimilation run, and $\mathrm{RMSE_b}$ the RMSE of the [2] baseline run. The RMSE values are calculated both for the state variables and the discharges. A positive value indicates an increase in RMSE as compared to the baseline run, a negative value a decrease. If observation and forecast bias are not taken into account, the analyzed discharge tends to be better estimated than for the baseline run, but this does not necessarily mean that the storages are better estimated. In other words, better discharge forecasts do not necessarily lead to better estimates of state variables. On the other hand, when biases are taken into account, the state variables are better estimated as compared to the baseline run (except for S). This leads also to better discharge estimates, as compared to the results of a bias-unaware EnKF.

7.4 State and bias estimation for a temporally variable observation and forecast bias

Figure 7 shows the comparison of the modeled storages to the synthetic truth for the three experiments with a [3] sinusoidally evolving observation and forecast bias. Figure 8 shows the comparison of the modeled discharge to the synthetic truth and the evolution of the observation bias. The same conclusions can be drawn as for the experiments with a constant observation bias. In all cases the observation bias and the discharge are better estimated with a bias-aware EnKF, as compared to when a bias-unaware EnKF is used. The estimation of the storages also strongly improves when a bias-aware EnKF is used, as opposed to the use of the bias-unaware EnKF. The only exception

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with reasonable accuracy

Number: 2 Author: Subject: Highlight Date: 6/17/13 10:28:08 PM

It is not clear what the "baseline run" is. Please explain.

Number: 3 Author: Subject: Highlight Date: 6/17/13 10:26:10 PM

What would be a physical explanation of such a bias? Would they be like biases that are periodical in nature? While I can understand observations can suffer from systematic instrument errors that are "seasonal", I cannot think of a model bias that would be periodical. Could you please elaborate a bit more on the nature of these assumptions?

is the estimation of S for experiment 3, where the bias and the RMSE slightly worsen. However, this storage does not directly influence the discharge, which explains the almost perfect estimation of the discharge.

Similar as for a constant observation bias, the results from experiment 2 and experiment 3 are almost identical when a bias-aware EnKF is used, but not when a bias-unaware EnKF is used. This can be explained by the relatively accurate estimation of the observation bias.

Table 3 shows that, for the comparison of the results to the results of the baseline run, the same conclusions can be drawn as for temporally constant observation and forecast biases. If biases are not taken into account, slightly better discharge estimates than the baseline run are obtained, with not necessarily better state estimates (except for experiment 3 where the discharge estimates are also worsened). Taking into account the biases again leads to better state estimates (except for the storage S).

7.5 Benefit of dual observation-forecast bias estimation

In order to demonstrate the benefit of the estimation of both forecast and observation biases, as opposed to the estimation of forecast biases alone (Dee and Da Silva, 1998; Dee and Todling, 2000; Drécourt et al., 2006; De Lannoy et al., 2007; Bosilovich et al., 2007; Reichle et al., 2010), the experiments described above were repeated, but the estimation of the observation bias was turned off. Under these conditions, the state and forecast bias estimation reduces to the methodology described in De Lannoy et al. (2007). Table 4 shows the results of the comparison of the analyzed storages and discharges to the synthetic truth. These statistics can be compared to the statistics in Figs. 5–8, in order to assess whether the estimation of both forecast and observation biases leads to better results than the estimation of forecast bias alone.

In all cases, as expected, the incorporation of an observation bias estimation leads to a better estimate of the states and discharges. This is expressed by the lower bias and RMSE values in Figs. 5–8 than in Table 4. These results thus clearly show the benefit of a dual state and observation and forecast bias estimation.

7.6 Analysis of the ensemble spread

A very important aspect of the application of the Kalman filter is to ensure an adequate ensemble spread. Figure 9 shows the square root of the diagonal elements of the biased a priori error covariance matrix (thus the ensemble spread) and the observation error covariance for the case with a sinusoidal observation and forecast bias. From these plots the conclusion can be drawn that the ensemble spread is stable throughout the simulation, and that ensemble collapse or instability do not occur. For the other experiments, similar results were obtained. Figure 10 shows the relationship between these ensemble spreads and the simulated discharge. The surface storage is only slightly correlated to the total discharge, while the spread in the surface and groundwater reservoir storages is more strongly correlated to the total discharge. As can be expected, the standard deviation of the observation bias is strongly correlated to the total discharge.

7.7 1 bservability of the biases

An important aspect in the application of the Kalman filter is the observability of the system. This can be examined through the 2 bservability matrix, of which the rank needs to be equal to the number of state variables. Since we are using persistent bias models, with less observations than the number of state variables, the rank of the observability matrix for the bias vectors will always be smaller than the number of state variables. In other words, the use of persistent bias models will always lead to an unobservable system. However, this observability issue is bypassed by the use of the parameters γ and κ in Eq. (24) and κ in Eq. (25), respectively. What these parameters essentially perform, is firstly separate the biased background error covariance into an error covariance of the unbiased states and an error covariance of the forecast bias, and secondly relate the biased background error covariance to the observation bias error covariance. If these two parameters are well chosen, by examining the correlation length of the innovations, one should expect an adequate partitioning of the mismatch between

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This sub-section does not really discuss any of the results presented in Section 7. The points that are being made are truly more general in nature, than just specific of the test cases being considered. I suggest merging Section 7.7 into Section 3.3.

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Please explain what the observability matrix is (for the readers that are not expert of data assimilation algorithms).

observations and simulations into biases and state variables. This is demonstrated by the results in the sections above. The development of realistic bias models is under investigation, but this subject falls outside the scope of this paper.

7.8 Assimilation of in situ discharge data

In order to demonstrate the applicability of the dual bias estimation in real-world situations, in situ observed discharge rates are assimilated instead of synthetically true values. Again, an observation error standard deviation of 0.1 $m^3 s^{-1}$ has been assumed, and an assimilation interval of 7 days has been used. Persistent bias models are again used. Figure 11 shows the results of this experiment. A seasonal cycle in the observation bias can be seen. This is very realistic, because there is a relatively large scatter in the discharge-water level relationship that is used to invert the water level observations into discharge values (W. Defloor, Department of Operational Water Management, Flemish Environmental Agency, personal communication, 2012). Since the water levels are usually low in the summer and high in the winter, this could lead to a seasonal signal in the observation bias. The bias in the storages evolves to realistic values. The unbiased discharge estimates and observations also show a slightly better match than the biased values, which increases confidence in the obtained results. This real-world application shows, at least for this relatively simple model, that the methodology can also be used in realistic situations.

8 Discussion and conclusions

In this paper, we presented a two-stage hybrid Kalman filter for the simultaneous estimation of forecast and observation biases and model state variables using the EnKF. The filter equations were first derived for a linear system. A first step consists of the updating of the forecast and observation biases, which are then used to update the unbiased state estimates. The Kalman gains for the forecast bias, the observation

bias, and the model state variables can be interpreted as the fraction of the mismatch between the observations and the corresponding model simulations that can be attributed to forecast bias, observation bias, and random forecast and observation error, respectively, remapping this mismatch onto state space for the model state and bias estimates.

The equations were then modified for nonlinear processes and observation systems in an ensemble framework. We followed the same approach as in De Lannoy et al. (2007). More specifically, a hydrid approach between an EnKF and a Discrete KF is suggested, in which the state vector is estimated using the EnKF, and the biases are estimated using the Discrete KF. The unbiased forecast error covariance and the forecast bias error covariance are calculated as fractions of the biased forecast error covariance. The observation bias error covariance is calculated as a multiplication of the observation prediction error covariance.

The developed methodology was then applied to a ~~very simple conceptual~~ rainfall-runoff model, in a situation with either only observation bias, both observation and forecast bias, or only forecast bias. The bias-aware EnKF with both observation and forecast bias estimation outperformed the bias-unaware EnKF, as well as the bias-aware EnKF with forecast bias estimation only.

The filter depends on two parameters, γ and κ, which are assumed constant in time, and which are used to estimate the bias error covariances. κ has been estimated by examining the temporal evolution of the forecast bias. For low values of κ, a continuous absolute growth of the forecast and observation bias was observed. The results were found to be less sensitive to the values for γ. It can be argued that these parameters should be made temporally variable, thus that a model for these two parameters would have to be developed. A more realistic model for the evolution of the biases could also be developed. Although this could certainly be the subject of further investigations, this falls outside the scope of this paper.

A next step in the development of the two-stage hybrid filter will be the assimilation of remotely sensed data such as soil moisture values into a spatially distribued,

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I found this example not adequately presented and documented. Fonts in Figure 11 are very small and, consequently, the results are hard to read and understand. The Authors should consider either expanding the presentation of this example, or removing it completely, leaving the application of the two-stage KF framework for this site to a future peer-review submission.

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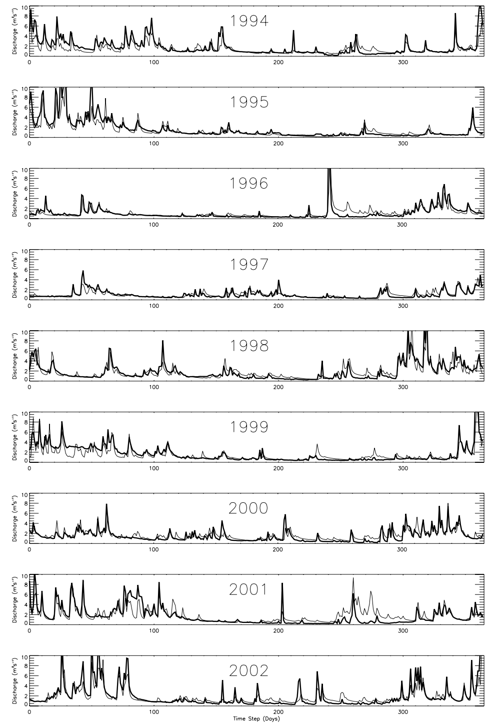

Fig. 2. Evaluation of the modeled discharge. The thick solid lines are the observed discharge, and the thin lines are the model results.

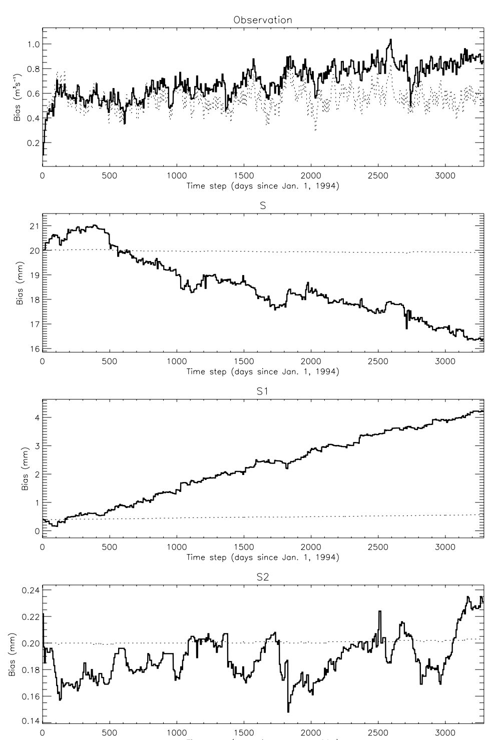

Fig. 3. Evolution of the estimated biases (the type of bias is indicated at the top of each plot) for experiment 2 using a multiplication factor (κ) of 10 (solid lines) and 100 (dotted lines) to calculate the observation bias error covariance.

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All figures, with the exception of Figures 2 and 4, are low quality, with very small fonts and hard to read. The Authors are invited to improve these Figures altogether and provide in the narrative of Section 7 and its subsections a more detailed description of the results and the significance of the results that are presented in these figures.