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The importance of state transformations when using the ensemble Kalman filter for unsaturated flow modeling: Dealing with strong nonlinearities

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ABSTRACT

The ensemble Kalman filter is, due to its computational efficiency, becoming more and more popular as a method for estimating both model states and parameters in hydrologic modeling, also for nonlinear state propagation models. In the ensemble Kalman filter the calculation of the error correlations, and hence the filter update, is done based on the ensemble of model evaluations and can therefore be strongly influenced by a few ensemble members with extreme values. With nonlinear state propagation models, extreme values can be a common phenomenon that can be, especially if there are nonlinearities between the observed variable and the modeled states, problematic during the filter update. An illustrative example of this problem is shown using an unsaturated flow model where the modeled states are pressure heads and observations are water content. It is demonstrated that the ensemble Kalman filter can in this case yield a deterioration of state predictions. We discuss the normal score transform and the transform with the retention function applied to the model states in order to mitigate this problem. It is shown that both transforms improve the estimation of the model states and parameters.

1. Introduction

Predictions, such as weather forecast or flood forecast, are usually made with numerical models. These models make predictions of states (for example, water or air pressure or temperature) at a certain time, based on initial conditions, model parameters, boundary conditions and forcing. With rapidly increasing power of numerical models, computer power and observation methods, these models get larger and more and more complex. Models that describe processes in large coupled systems of compartments, such as soils, aquifers and land surface, to make predictions of fluxes in the system, are now available [26,32]. Predictions are optimized by integrating observations (data assimilation [37]). The balance between efficiency and model quality is a challenge when setting up data assimilation schemes for large models. The Kalman filter or ensemble Kalman filter [16] is a very popular scheme for this purpose. It is used for hydrologic predictions [11,38,45], reservoir modeling [21,30,35,47] and weather prediction [1,24], among many others.

Using the Kalman filter in prediction models, the model states (and possibly parameters or boundary and forcing data) are updated sequentially in time with observation series, where the update depends on the correlation between state and observation prediction errors. In the ensemble Kalman filter, the means and error correlations are approximated from the first and second moments of an ensemble of state variables, which makes it applicable to non-linear models. The method is described in more detail in Section 2.2. Its advantages for large models are strong: It is very efficient, relatively simple to implement and to extend. The Kalman filter is an exact method for linear models with Gaussian noise terms, while it is always an approximation for non-linear problems with non-Gaussian noise.

In the applications described above, the state propagation models are usually strongly non-linear, highly uncertain in terms of parameters and boundary conditions and they are subject to modeling errors in the sense that not all relevant processes are captured by the model. Also, uncertainties are hardly ever Gaussian, but often have strong tailing and restricted ranges (e.g. [4]). Nevertheless, application of the EnKF has been shown to be very successful in many applications (for example [31]).

The ensemble Kalman filter is also used for subsurface flow models [6,36], which are then often not stand alone, but part of a larger system. For example, flow in the subsurface can be modeled as a part of land surface models. The purpose of modeling is then mainly the state prediction, rather than parameter identification. It should be

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noted that the ensemble Kalman filter is also used as a method to estimate heterogeneously distributed parameter fields (in most cases saturated hydraulic conductivity) in groundwater flow or reservoir modeling (for example [23,25,29,30,49]).

The important subsurface part in land surface models is the unsaturated zone. The transport of water in the unsaturated zone is described by a mass balance for water. The water fluxes are described by the Buckingham–Darcy equation. The model requires two constitutive relations. It is non-linear, the distributions of water content and pressure head values as well as soil parameter distributions are often non-Gaussian and it is as a model type strongly debated among soil scientists [13,22,27], as it makes strong simplifications of processes that are known to be often not justified. An example is hysteretic behavior of the constitutive relations that is usually not captured in models. Therefore, modeling error in this sense has to be expected in applications. The non-linearity comes very prominently to play when water content (or soil moisture) observations are used. These are popular observations, as they can be obtained from remote sensing data or from permanently installed devices, such as TDR probes [34]. However, the primary variable in the standard model is the water pressure head. The water pressure head has in principle a range from plus to minus infinity, even if the extreme values are physically not reasonable. The retention function (one constitutive relation of the model) describes the water content as a function of the water pressure head, which we assume here to be unique (meaning we neglect hysteresis). It is usually highly nonlinear. It maps the extreme values of the negative pressure heads to a very small range of values of the water content and all positive pressure heads to the saturated water content.

The ensemble Kalman filter has been tested for unsaturated zone models for its performance for parameter identification and prediction [28,48]. Despite the non-ideal properties of unsaturated flow models, these studies concluded that the method worked successfully. However, the studies used synthetic test cases where the assimilation model was the same type as the model that generated the data and/or used pressure heads as observations, which avoids parts of the problem of the non-linear mapping. The ensemble Kalman filter has also been applied successfully to studies on estimation of heterogeneous parameter fields, which were also synthetic and focused on the saturated hydraulic conductivity parameter only [44]. Naturally, the ensemble Kalman filter has been used often for unsaturated zone models in practice with great success [9,10]. In these studies, however, the focus was on the (observed) soil moisture and the land surface processes and less on the pressure heads as primary variables of the Richards equation.

Although there are many examples where the ensemble Kalman filter has been successfully applied in unsaturated flow models, it needs to be tested carefully before application, as the flow model is very nonlinear. This comes to play, for example, if water pressure head is needed as state variable. Although the water pressure head is not directly relevant in the water budget (for which the models are mostly used), it plays an important indirect role. In a land surface model, the limitation for evaporation from the soil surface as well as the wilting of plants and limitation of plant root water uptake under dry conditions is linked directly to the water pressure head. Also, if aquifers and unsaturated zone should be described in one model, the pressure head has to be considered for the aquifer part, where water content is always equal to one. The pressure head plays also an important role for technical matters. For example, bias corrections might be used in the ensemble Kalman filter to account for non-resolved soil structure, such as layering [15]. The bias correction is best applied to the pressure head, as its effect on the water content is limited.

As the ensemble Kalman filter works ideally for linear systems with Gaussian noise, it can be beneficial to implement it into a model at a place and in a way where these conditions are violated least. This point is demonstrated in this paper for an unsaturated zone model where water content is observed, but water pressure head is the variable of interest. The nonlinear state propagation model combined with the model uncertainty that is characteristic for unsaturated flow can cause large errors if the ensemble Kalman filter is applied in a standard form. We demonstrate this with a test case that is set up to focus on this issue. We also demonstrate that the performance of the filter can be strongly improved if the filter is set up such that non-linearity is dampened, even if the model is uncertain in the sense that it might not capture all processes. This is done with a normal score (NS) transform and alternatively with the water content–pressure head relation as a mapping. Normal score transformation (e.g. [12,20]) transfers a non-Gaussian state variable into a Gaussian one analytically or numerically. The application of NS in EnKF is well established in oceanography [2,3,42,43], reservoir modeling [21] and subsurface hydrology [29,41,49]. In subsurface hydrology, the goal was always to identify heterogeneous parameter fields. Though a number of demonstrations are available to show the applicability and advantage of NS-EnKF in groundwater studies, to our best knowledge, the application of NS-EnKF is not available in unsaturated zone studies. No studies, mentioned in the above paragraph, handled the non Gaussian state distribution during the analysis step of EnKF. The different transformation schemes are discussed and compared in Section 4. Before this, the model and the filter scheme are outlined in Section 2, while the problem described above is demonstrated in Section 3. Discussion and conclusions are given in Section 5.

2. Theory and background

2.1. Unsaturated flow modeling

Flow in the unsaturated zone is commonly described by the Richards equation [39], here given in the mixed formulation in 1D:

$$\frac{\partial\Theta}{\partial t} - \frac{\partial}{\partial z}\left(K_{\text{sat}}K_{\text{rel}}(h)\left(\frac{\partial h}{\partial z}+1\right)\right) = 0 \tag{1}$$

where Θ is the volumetric water content (m^3/m^3), K_{sat} is the saturated hydraulic conductivity (m/s), K_{rel} the relative permeability (−), h the water pressure head (m). Commonly for variably saturated flow, the pressure based or the mixed formulations with pressure head as primary variable are used in numerical implementations. Formulations with water content as primary variable cannot handle full saturation well and are therefore more restricted in terms of usage. For the Richards equation, the relation between the pressure head and the water content as well as between the pressure head and the relative permeability must be prescribed. In this work, two parameterizations are considered for this purpose. The first is the simple exponential model of Russo [40] and Gardner [18] with one parameter:

$$\Theta(h) = \Theta_r + (\Theta_s - \Theta_r)[e^{-0.5\alpha_{GR}|h|}(1+0.5\alpha_{GR}|h|)]^{2/2.5} \tag{2a}$$

$$K_{\text{rel}}(h) = e^{-\alpha_{GR}|h|} \tag{2b}$$

where Θ_s is the saturated water content (equaling the porosity), Θ_r the residual water content and α (m^{-1}) the pore size distribution parameter. The second is the more complex parameterization of [46], which has two parameters and is very commonly used:

$$\Theta(h) = \Theta_r + \frac{\Theta_s - \Theta_r}{\left[1+(\alpha_{VG}|h|)^n\right]^m} \tag{3a}$$

$$K_{\text{rel}}(h) = [1-(1-S_e^{1/m})^m]^2 S_e^{0.5} \tag{3b}$$

where $S_e = (\Theta - \Theta_r)/(\Theta_s - \Theta_r)$, n (−) and m are shape parameters and $m = 1 + 1/n$. For the state propagation models used in this work, the van Genuchten (VG) parameterization is used for the synthetic truth, while the Russo–Gardner (RG) parameterization is only used for EnKF simulations.