Uncertainty assessment of hydrologic model states and parameters: Sequential data assimilation using the particle filter

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[1] Two elementary issues in contemporary Earth system science and engineering are (1) the specification of model parameter values which characterize a system and (2) the estimation of state variables which express the system dynamic. This paper explores a novel sequential hydrologic data assimilation approach for estimating model parameters and state variables using particle filters (PFs). PFs have their origin in Bayesian estimation. Methods for batch calibration, despite major recent advances, appear to lack the flexibility required to treat uncertainties in the current system as new information is received. Methods based on sequential Bayesian estimation seem better able to take advantage of the temporal organization and structure of information, so that better compliance of the model output with observations can be achieved. Such methods provide platforms for improved uncertainty assessment and estimation of hydrologic model components, by providing more complete and accurate representations of the forecast and analysis probability distributions. This paper introduces particle filtering as a sequential Bayesian filtering having features that represent the full probability distribution of predictive uncertainties. Particle filters have, so far, generally been used to recursively estimate the posterior distribution of the model state; this paper investigates their applicability to the approximation of the posterior distribution of parameters. The capability and usefulness of particle filters for adaptive inference of the joint posterior distribution of the parameters and state variables are illustrated via two case studies using a parsimonious conceptual hydrologic model.

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1. Introduction and Scope

[2] Hydrologic models, from the simplest to the most complex, are often used to predict the future evolution of variables of interest based on modeled estimates of the current states and parameters of the system. However, a long-standing problem in hydrology has been how to retrieve estimates of system states and parameters for a given domain (e.g., land surface) using measurements made on system fluxes and other quantities. The hydrologic system involves complex interactions among the atmospheric, land surface, and subsurface components of the water cycle. Hydrologic models typically conceptualize and represent these complex behaviors using relatively simple mathematical equations in which the (conceptualized) model parameters are aggregate quantities representing spatial and temporal properties of the system and are generally not directly and easily measurable in the field; they must therefore be inferred by indirect methods such as model calibration [*Gupta et al.*, 1998]. A variety of model calibration techniques have been developed to ensure consistency between the model simulations of system behavior and their corresponding observations (see *Duan et al.* [2003] for a comprehensive review). The most elementary approach, manual calibration, is performed by visual inspection of the agreement and differences between model predictions and the observations for some historical period of record, with analysis of the differences used to guide trial-and-error adjustments of the model parameters [*Boyle et al.*, 2000; *Gupta et al.*, 2003a]. The subjectivity and time-consuming nature of manual model calibration has motivated the development of automatic calibration techniques [*Sorooshian and Dracup*, 1980; *Duan et al.*, 1992; *Beven and Binley*, 1992; *Sorooshian et al.*, 1993; *Gupta et al.*, 1998]. However,

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despite major progress, automated calibration techniques still lack the capability to properly treat the various uncertainties inherent in the system. Studies using a number of interesting methods, rooted in both classical Bayesian estimation and the more contemporary multicriteria approach, have shown how they can be used to quantify the inability of the model to generate precise and accurate forecasts that properly reflect model parameter and predictive uncertainty [*Kuczera*, 1983; *Beven and Binley*, 1992; *Kuczera and Parent*, 1998; *Yapo et al.*, 1998; *Gupta et al.*, 1998; *Boyle et al.*, 2000; *Kavetski et al.*, 2003; *Vrugt et al.*, 2003]. Such methods typically rely on one or more aggregate statistical measures to measure and minimize the long-term prediction error over some historical period of calibration and validation data, by implicitly (or explicitly) assuming time-invariance of the parameters. Major weaknesses of such ''batch'' calibration procedures include (1) the requirement that a set of historical data be collected and maintained in storage to be processed en masse results in computational burden, (2) batch processing of data diminishes flexibility and complicates the investigation of possible temporal variations in the model parameters, and (3) in the case of insufficient availability of historical data (e.g., ungauged or recently gauged basins) batch methods cannot be properly applied.

[3] Considering that initial conditions such as water and heat storages cause the memory effect in the hydrologic system, sequential data assimilation can improve hydrologic predictability by taking the best advantage of information content. Several authors have suggested the need to adopt sequential estimation methods to strengthen model calibration by improving the assimilation of information from observations. Sequential techniques reported in the hydrologic literature include the dynamic identifiability analysis (DYNIA) for recursive evaluation of the identifiability and time variability of parameters [*Wagener et al.*, 2003], data-based mechanistic modeling involving recursive estimation of time-varying parameters [*Young*, 2001], the parameter estimation method based on the localization of information (PIMLI) approach of *Vrugt et al.* [2002], and Bayesian recursive estimation (BaRE) for estimating parameter and predictive uncertainty for conceptual hydrologic models [*Thiemann et al.*, 2001; *Misirli et al.*, 2003]. The BaRE algorithm employs a recursive Bayesian scheme for investigating the conditional probability distribution (reported using 95% confidence bounds) of interacting model parameters. The major problem with the initial version of this algorithm [see *Beven and Young*, 2003; *Gupta et al.*, 2003b] was its tendency to convergence to a single point estimate, a drawback corrected by *Misirli* [2003]. We refer to this phenomenon as degeneracy (see section 3.2) and will discuss the important role of resampling to avoid this problem. Other sequential estimation strategies include the standard Kalman filter algorithm applied to real time streamflow forecasting [*Todini et al.*, 1976; *Kitanidis and Bras*, 1980a, 1980b; *Bras and Restrepo-Posada*, 1980; *Bras and Rodriguez-Iturbe*, 1985; *Awwad and Valdés*, 1992; *Awwad et al.*, 1994; *Young*, 2002], recursive estimation of model parameters for water quality models [*Beck*, 1987], and the ensemble Kalman filter (EnKF) for dual estimation of states and parameters and also the predictive uncertainty bounds in conceptual hydrologic models [*Moradkhani et al.*, 2005].

[4] While the various Kalman filter–based recursive procedures are relatively simple to implement and have nice properties, the evolution of the filter is governed by its second-order characteristics and a linear correction (updating) procedure. However, because the state variables in stochastic-dynamic systems are modeled as random variables, subject to unknown disturbances, the conditional probability of the prediction will translate, deform, and spread, and the shape of this distribution is difficult to track for models having strongly nonlinear behavior. For such cases, an accurate computation of prediction probabilities requires the tracking of higher-order moments. Recent developments in sequential Monte Carlo (SMC) methods [*Gordon et al.*, 1993; *Fruhwirth-Schnatter*, 1994; *Cargnoni et al.*, 1997; *Liu and Chen*, 1998; *Doucet et al.*, 2001; *Pham*, 2001; *Arulampalam et al.*, 2002] now make the application of such methods attainable for the uncertainty assessment of hydrologic models. SMC methods, also known as particle filters, have garnered considerable attention among researchers in communication theory, signal processing, and target tracking [*Djurić et al.*, 2003]. These methods allow for a relatively complete representation of the posterior distribution so that system nonlinearities can easily be handled and the statistical characteristics of the distributions (e.g., mean, mode, kurtosis, variance, etc.) can readily be computed. Perhaps the earliest applications of Monte Carlo methods for statistical inference are given by *Handschin* [1970], *Akashi and Kumamoto* [1975], and *Zaritskii et al.* [1975], but the formal particle filter approach was established by *Gordon et al.* [1993] through the introduction of a novel resampling technique.

[5] This paper is organized as follows. Section 2 discusses sequential Bayesian data assimilation in the context of a simple state-space model formulation and describes the formal methodology required for Bayesian filtering. We discuss the intractability of the formal sequential Bayesian approach in section 3 and present the Monte Carlo procedure known as particle filtering, which uses sequential importance sampling (SIS) and sampling importance resampling (SIR). The improvement in the filter's performance due to resampling is illustrated using an example. Although particle filters have generally been applied to estimation of the dynamic states in a system, we discuss their applicability to static state (parameter) estimation. In previous work we have explored the same problem using a dual EnKF approach [*Moradkhani et al.*, 2005], which tracks only the first two moments of the distributions; the important difference here is that particle filters use a full Bayesian updating (correction) scheme. In section 4, two case studies demonstrating the performance of the filter for hydrologic modeling (using a parsimonious conceptual rainfall-runoff model) are presented. In the first case, a synthetic study is used to demonstrate the capability of a particle filter for estimating known parameter and state posterior distributions. The second case applies the particle filter to the real-world problem of assimilating historical streamflow data for improving streamflow forecasts. Section 5 summarizes the methodology and dis-

cusses possibilities for its improvement and application to other hydrologic data assimilation problems.

2. Sequential Bayesian Data Assimilation

2.1. Limitations of the Procedures Rooted in Kalman Filter

[6] For a linear stochastic-dynamical system, it is possible to derive an exact analytical expression for recursive calculation of the posterior distribution of simulated variables using the celebrated Kalman filter [*Kalman*, 1960]. Under certain conditions, the method can be extended to the nonlinear case by linearizing the model around the current estimate of the state vector, using the approach known as the extended Kalman filter (EKF) [*Jazwinski*, 1970; *Reichle et al.*, 2002a]. However, the major limitation of Kalman filter and its extensions are their closure at the second-order moments, implying that filter evolution is uniquely determined by their second-order characteristics. The EKF, in particular, has many well-known drawbacks, including the high computational demand required for propagation of the error covariance and the closure approximation arising from neglecting the higher-order derivatives of the model; the EKF is therefore susceptible to divergence and instability [*Jazwinski*, 1970; *Bras and Rodriguez-Iturbe*, 1985; *Gauthier et al.*, 1993; *Miller et al.*, 1994].

[7] The ensemble Kalman filter (EnKF) was introduced by *Evensen* [1994] and clarified by *Burgers et al.* [1998] and *Van Leeuwen* [1999] as a means of addressing the above mentioned difficulties encountered in the nonlinear filtering problem. The EnKF uses a Monte Carlo approach to approximate the conditional second-order moments of interest using a finite number of randomly generated model trajectories but also has the aforementioned limitations. To improve accuracy and stability, and to obtain correct estimates of prediction uncertainty, it is important to track the time evolution of the model by means of all moment characteristics through a full probability density function. This becomes possible when the sequential Bayesian scheme is employed.

2.2. Generic State-Space Model

[8] Over the course of the past decade, Earth system science data assimilation activities have rapidly increased, attracting the attention of hydrologists seeking to exploit the potential use of real-time observations for producing more accurate hydrological forecasts [*McLaughlin*, 1995; *Reichle et al.*, 2002a, 2002b; *McLaughlin*, 2002; *Young*, 2002; *Troch et al.*, 2003]. Sequential data assimilation consists of a process whereby the system state is recursively estimated/corrected each time an observation becomes available. Consider the following generic dynamic state-space formulation of a stochastic model:

$$x_{k+1} = f(x_k, \theta, u_k) + \omega_{k+1} \qquad \omega_{k+1} \sim N(0, Q_{k+1}), \tag{1}$$

where $x_k \in \Re^{N_x}$ is an N_x-dimensional vector representing the system state (for example, catchment soil moisture content) at time t_k. The nonlinear operator f: $\Re^{N_x} \rightarrow \Re^{N_x}$ expresses the system transition from time t_k to t_{k+1} in response to the model input vector (forcing data, u_k, e.g., mean areal precipitation). θ represents the vector of time-invariant model parameters, and ω_{k+1} is viewed as a white noise random sequence in the discrete-time domain with mean zero and variance Q_{k+1}.

[9] Suppose that a set of scalar observations is taken at time t_{k+1} and we intend to assimilate the vector of observations into the model. The output variables of the model are functions of both the model state variables and the parameters characterizing the model. The observation process in general form can be written as

$$y_{k+1} = h(x_{k+1}, \theta) + \nu_{k+1} \qquad \nu_{k+1} \sim N(0, R_{k+1}), \tag{2}$$

where $y_{k+1} \in \Re^{N_y}$ is an N_y-dimensional observation vector (observation simulation, e.g., streamflow) as a function of model parameters and forecasted state variables through the nonlinear operator h: $\Re^{N_x} \rightarrow \Re^{N_y}$. Here ν_{k+1} is the observational white random noise with mean zero and variance R_{k+1}. The noise terms of ω_{k+1} and ν_{k+1} are generally assumed to be independent random vectors.

2.3. Sequential Bayesian Filtering Formalism

[10] Discrete dynamic state-space models lend themselves naturally to Bayesian analysis. In this setting, a new inference is drawn at each time t_k by assimilating information from the available observations $y_1, \ldots, y_k$. More specifically, at time t_k a sequential analysis may seek to estimate past states $x_1, x_2, \ldots, x_{k-1}$ (smoothing), the current state x_k (filtering), or the next state x_{k+1} (forecast). Because of its stochastic nature, x_k is a random variable; hence all pertinent information about $x_1, x_2, \ldots, x_k$ given observations up to time k can be extracted from the posterior distribution $p(x_{1:k}|y_{1:k})$. Our current study seeks to estimate this distribution recursively in time, with particular interest in the marginal distribution, the so-called filtering posterior $p(x_k|y_{1:k})$. Given the filtering posterior, one can easily calculate the desired point (mode or mean) or interval estimates of the system state and output. This is known as the "Bayesian filtering problem" or "optimal filtering." The state posterior distribution at time t_k is given by Bayes' theorem as

$$p(x_{0:k+1}|y_{1:k+1}) = \frac{p(y_{1:k+1}|x_{0:k+1})p(x_{0:k+1})}{p(y_{1:k+1})}, \tag{3}$$

where, $p(y_{1:k+1}|x_{0:k+1})$ is the likelihood, $p(x_{0:k+1})$ is the prior, and $p(y_{1:k+1})$ is the normalization factor.

[11] It is straightforward to obtain the recursive form of the posterior as follows:

$$p(x_{0:k+1}|y_{1:k+1}) = \frac{p(y_{k+1}|x_{0:k+1}|y_{1:k})p(x_{0:k+1}|y_{1:k})}{p(y_{k+1}|y_{1:k})}. \tag{4}$$

The conditional distribution at (4) summarizes all the information available about the stochastic-dynamic system represented by (1).

[12] The filtering posterior distribution $p(x_{k+1}|y_{1:k+1})$ can also be written as

$$p(x_{k+1}|y_{1:k+1}) = \frac{p(y_{k+1}|x_{k+1})p(x_{k+1}|y_{1:k})}{p(y_{k+1}|y_{1:k})}. \tag{5}$$

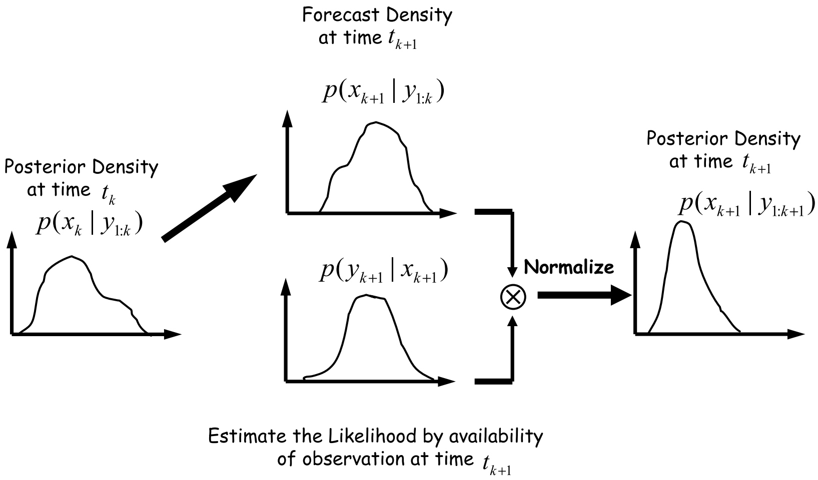

Figure 1. Formal Bayesian scheme for evolution of the conditional probability density of the state variables by assimilating observations from time t_k to time t_{k+1}.

Using the total probability, the forecast density $p(x_{k+1}|y_{1:k})$ is obtained via the Chapman-Kolmogorov equation

$$p(x_{k+1}|y_{1:k}) = \int_{x_k} p(x_{k+1}|x_k, y_{1:k})p(x_k|y_{1:k})dx_k. \quad (6)$$

Given the Markovian property of order one in equation (1), that is, system state at each time step is just dependent on the previous state, the forecast density simplifies to

$$p(x_{k+1}|y_{1:k}) = \int_{x_k} p(x_{k+1}|x_k)p(x_k|y_{1:k})dx_k. \quad (7)$$

Figure 1 displays a schematic of the sequential Bayesian scheme (equation (5)). The probabilistic model for evolution of the state is defined by the system equation (1) with the assumption of Gaussian system noise having variance Q_k. The transition probability $p(x_{k+1}|x_k)$ at time t_{k+1} is written as $p(x_{k+1} - f_k()|Q_k)$. The normalizing factor, known as predictive distribution or evidence, is written as follows:

$$p(y_{k+1}|y_{1:k}) = \int_{x_{k+1}} p(y_{k+1}|x_{k+1})p(x_{k+1}|y_{1:k})dx_{k+1}. \quad (8)$$

By assuming Gaussian observation noise having variance R_{k+1}, the likelihood $p(y_{k+1}|x_{k+1})$ at time t_{k+1} can be represented as $p(y_{k+1} - h_{k+1}()|R_{k+1})$, where $p(\nu|R) = \exp(-\frac{1}{2}\nu^T R^{-1}\nu)/\sqrt{\det(2\pi R)}$ represents the Gaussian distribution at ν with mean zero and variance R. Assuming that observation noises are heteroscedastic (variance changing) [*Sorooshian and Dracup*, 1980] and uncorrelated, we assume the variance of the noise to be proportional to the magnitude of the observations, represented as $R_{k+1} = \rho \, . \, y_{k+1}$, where ρ is the proportionality factor determining the spread of the likelihood function (for details, see *Moradkhani et al.* [2005]). By substituting the likelihood (as mentioned above) in (5) and combining it with (7) and (8), the update step (filtering posterior) is written as

$$p(x_{k+1}|y_{1:k+1}) = \frac{p(y_{k+1} - h_{k+1}()|R_{k+1}) \int p(x_{k+1} - f_k()|Q_k)p(x_k|y_{1:k})dx_k}{\int [p(y_{k+1} - h_{k+1}()|R_{k+1})] \left[\int p(x_{k+1} - f_k()|Q_k)p(x_k|y_{1:k})dx_k \right] dx_{k+1}} \quad (9)$$

[13] Although this recursive form presents a nice conceptual representation of the method for filtering the posterior density of model state variables, the multidimensional integration typically makes a closed-form solution intractable for hydrologic systems. A more general tractable solution approach involves application of the sequential Monte Carlo (MC) sampling method [*Doucet et al.*, 2000].

3. Particle Filtering

3.1. Sequential Monte Carlo

[14] As mentioned earlier, in some specific cases a sequential analysis can be carried out using the analytical form of the filter (e.g., standard Kalman filter) thereby achieving exact calculations for the posterior distributions of interest. However, unlike the Kalman filter which simplifies recursive estimation by assuming Gaussian distributional properties for the prognostic (state) variables, Monte Carlo methods based on particle filters relax the need for restrictive assumptions regarding the forms of the probability densities; that is, they can handle the propagation of non-Gaussian distribution through nonlinear models. In essence, Monte Carlo simulation provides a straightforward approach for performing stochastic model computations by generating a large number of random realizations of the variables or parameters of interest, solving deterministic equations for each realization, and estimating the statistical properties of the results from the ensemble of realizations.

[15] The earliest application of SMC methods can be traced back to the 1950s in the field of polymer growth [*Hammersley and Morton*, 1954; *Rosenbluth and Rosenbluth*, 1956]. Although SMC methods found limited use in the beginning, the advent of high-speed computers during the past decade has led to widespread application of SMCs, and particularly particle filters have become a very active area of research. The particle filter is a SMC procedure developed principally to allow for a full representation of the probability distributions of state variables via a number of independent random samples called particles. The particles are sampled directly from the state-space to represent the posterior probability, and updated by assimilating the information contained in the new observations. Particles are properly located, weighted, and propagated sequentially by application of the Bayesian rule. The approach is also sometimes known as the bootstrap filter, condensation algorithm, interacting particle approximation, or survival of the fittest [*Gordon et al.*, 1993; *Carpenter et al.*, 1999; *Crisan et al.*, 1999; *Kanazawa et al.*, 1995; *Doucet et al.*, 2001]. In particle filtering, the posterior distributions are approximated by discrete random measures defined by particles and a set of weights associated with particles. The particles drawn from the posterior distribution at time t_{k+1} are used to map integrals to discrete sums by the following empirical approximation [*Arulampalam et al.*, 2002]:

$$p(x_{0:k+1}|y_{1:k+1}) = \sum_{i=1}^{N_p} w_{k+1}^i \delta\left(x_{0:k+1} - x_{0:k+1}^i\right), \tag{10}$$

where $\{x_{k+1}^i,\ w_{k+1}^i\}$ denote the ith particle and its weight, respectively, and $\delta()$ denotes the Direc delta function.

3.2. Sequential Importance Sampling (SIS)

[16] The important concept in particle filtering is the principle of (SIS) or Bayesian importance sampling (BIS), used for selection of the particle weights [*Doucet*, 1998]. The more commonly used SIS principle is based on the fact that direct sampling from the target density (posterior) $p(x_{0:k+1}|y_{1:k+1})$, which is often non-Gaussian, is generally difficult (if not impossible). To avoid this difficulty, importance sampling generates particles x_{k+1}^i from a known function $q(x_{0:k+1}|y_{1:k+1})$ known as a proposal distribution (or importance density) and assigns the weights (importance weights) according to

$$w_{k+1}^{i*} = \frac{p\left(x_{0:k+1}^i|y_{1:k+1}\right)}{q\left(x_{0:k+1}^i|y_{1:k+1}\right)}. \tag{11}$$

A sequential update to the importance weights, at each iteration, is achieved by factorizing the proposal distribution such that

$$q(x_{0:k+1}|y_{1:k+1}) = q(x_{k+1}|x_{0:k}, y_{1:k+1})q(x_{0:k}|y_{1:k}). \tag{12}$$

Using this relation, the new sample $x_{k+1}^i \sim q(x_{k+1}|x_{0:k}, y_{1:k+1})$ is augmented to the existing samples $x_{0:k}^i \sim q(x_{0:k}|y_{1:k})$ to obtain the samples $x_{0:k+1}^i \sim q(x_{0:k+1}|y_{1:k+1})$. To derive the weight updating equation, we simplify (4) as

$$\begin{aligned} p(x_{0:k+1}|y_{1:k+1}) &= \frac{p(y_{k+1}|x_{k+1}|y_{1:k})p(x_{k+1}|x_k)}{p(y_{k+1}|y_{1:k})}p(x_{0:k}|y_{1:k}) \\ &\propto p(y_{k+1}|x_{k+1}|y_{1:k})p(x_{k+1}|x_k)p(x_{0:k}|y_{1:k}). \end{aligned} \tag{13}$$

By substituting (12) and (13) into (11), a sequential estimate for the importance weights is derived as

$$\begin{aligned} w_{k+1}^{i*} &\propto \frac{p\left(y_{k+1}|x_{k+1}^i|y_{1:k}\right)p\left(x_{k+1}^i|x_k^i\right)p\left(x_{0:k}^i|y_{1:k}\right)}{q\left(x_{k+1}^i|x_{0:k}^i, y_{1:k+1}\right)q\left(x_{0:k}^i|y_{1:k}\right)} \\ &= w_k^{i*}\frac{p\left(y_{k+1}|x_{k+1}^i|y_{1:k}\right)p\left(x_{k+1}^i|x_k^i\right)}{q\left(x_{k+1}^i|x_{0:k}^i, y_{1:k+1}\right)}. \end{aligned} \tag{14}$$

Equation (14) expresses the basic principle of the sequential importance sampling filter. *Arulampalam et al.* [2002] explained that if $q(x_{k+1}|x_{0:k},\ y_{1:k+1}) = q(x_{k+1}|x_k,\ y_{k+1})$, only x_{k+1}^i needs to be kept in storage, and therefore all the computed values of $x_{0:k}^i$ and history of observations $y_{1:k}$ are discarded and the weight updating simplifies to

$$w_{k+1}^{i*} \propto w_k^{i*}\frac{p\left(y_{k+1}|x_{k+1}^i\right)p\left(x_{k+1}^i|x_k^i\right)}{q\left(x_{k+1}^i|x_k^i, y_{k+1}\right)}. \tag{15}$$

Correspondingly, the filtering posterior density in (9) is approximated by

$$p(x_{k+1}|y_{1:k+1}) = \sum_{i=1}^{N_p} w_{k+1}^i \delta\left(x_{k+1} - x_{k+1}^i\right). \tag{16}$$

where w_{k+1}^i are the normalized weights given by

$$w_{k+1}^i = \frac{w_{k+1}^{i*}}{\sum_{i=1}^{N_p} w_{k+1}^{i*}}. \tag{17}$$

With such an approximation, any expectations with the complicated form of

$$\mathrm{E}[g(X)] = \int_{x_{k+1}} g(x_{k+1})p(x_{k+1}|y_{1:k+1})dx_{k+1} \tag{18}$$

may be approximated by

$$\mathrm{E}[g(X)] \approx \sum_{i=1}^{N_p} w_{k+1}^i g\left(x_{k+1}^i\right). \tag{19}$$

We therefore obtain a discrete weighted approximation to the true filtering posterior. By increasing the number of particles ($N_p \to \infty$), the estimate will converge to the true expectation.

[17] Several authors [*Doucet et al.*, 2000; *Wan and Van der Merwe*, 2001; *Arulampalam et al.*, 2002; *Djurić et al.*,

2003] have reported that the choice of proposal function is a critical design issue and one may achieve poor performance if the proposal function is not well chosen. The most convenient and frequently used importance function is the transition prior, where

$$q\left(x_{k+1}^i|x_k^i, y_{k+1}\right) = p\left(x_{k+1}|x_k^i\right). \tag{20}$$

By substituting (20) into (15), the weight updating becomes

$$w_{k+1}^{i*} \propto w_k^{i*} p\left(y_{k+1}|x_{k+1}^i\right). \tag{21}$$

[18] A common problem with the SIS particle filter, however, is that the performance of the filter deteriorates quickly due to degeneration of random measures. Degeneracy is an undesirable and unavoidable effect in SIS particle filters where the variance of the importance weights increases stochastically over time, occurring because after a few iteration (time steps), all the particles except one are discarded because their importance weights become insignificant [*Doucet*, 1998]. The effective sample size can be used as a measure of degeneracy [*Kong et al.*, 1994; *Liu and Chen*, 1998]; however, the exact effective sample size cannot be computed and we must therefore rely on an estimated value according to (22) (see *Doucet* [1998] for exact derivation of effective sample size).

$$N_{eff} \approx \frac{1}{\sum_{i=1}^{N_p} w_{k+1}^i} \tag{22}$$

[19] *Arulampalam et al.* [2002] explained that small N_{eff} indicates severe degeneracy, and therefore it is common to set a fixed threshold N_{thresh} so that if $N_{eff} \leq N_{thresh}$, the effect of degeneracy needs to be reduced by resampling. In practice, a resampling step is frequently essential for the filter to work [*Pham*, 2001]. In essence, resampling is followed by a Markov chain chaotic Monte Carlo (MCMC) move step, which introduces a sample variety without deteriorating the characterization of the posterior distribution. Several resampling schemes have been proposed in literature including sampling importance resampling [*Rubin*, 1988; *Smith and Gelfand*, 1992], residual resampling [*MacKay*, 1992; *Higuchi*, 1997], auxiliary sampling importance resampling [*Pitt and Shephard*, 1999], minimum variance sampling [*Doucet et al.*, 2001], and regularization based on kernel density [*Musso et al.*, 2001]. Next, we elaborate on the sampling importance resampling algorithm and will examine the applicability and usefulness of this procedure in hydrologic data assimilation.

3.3. Sampling Importance Resampling (SIR) Particle Filter

[20] In a generic particle filter (equations (10)–(17)), particles tend toward dispersion owing to the stochastic behavior of the system, with the result that many of them drift away from the "truth" and obtain negligible weight (probability); that is, only a few particles participate effectively in the filter. The SIR particle filter avoids this problem by adding a resampling procedure to the SIS particle filter [*Rubin*, 1988; *Smith and Gelfand*, 1992]. The SIR scheme eliminates particles having low importance weights while accumulating particles having high importance weight, essentially by mapping the Dirac random measure $\{x_k^i, w_k^i\}$ into an equally weighted random measure $\{x_k^i, 1/N_p\}$ so that N_p particles are produced all with weighting $1/N_p$. The SIR algorithm consists of two steps: (1) The importance density $q(x_{k+1}|x_k^i, y_{k+1})$ is chosen to be the prior transition density $p(x_{k+1}|x_k^i)$, and (2) resampling is performed as outlined in Figure 2. The SIS and SIR filters are very similar, with the only difference being that in SIR, resampling is always performed at each step, while in SIS, resampling is carried out when degeneracy occurs. The following one-dimensional state-space problem example is used to illustrate the reduction of degeneracy using SIR.

3.4. Problem: One-Dimensional State-Space Model

[21] Consider the application of SIS and SIR particle filtering to the following non-Gaussian, nonlinear state-space and observation model used as an illustrative example by several authors [*Andrade Netto et al.*, 1978; *Gordon et al.*, 1993; *Kitagawa*, 1996; *Doucet et al.*, 2000]:

$$x_k = \frac{1}{2}x_{k-1} + 25\frac{x_{k-1}}{1 + x_{k-1}^2} + 8\cos(1.2k) + \omega_k \quad \omega_k \sim N\left(0, \sigma_w^2\right) \tag{23}$$

$$y_k = \frac{x_k^2}{20} + \nu_k \qquad \nu_k \sim N\left(0, \sigma_\nu^2\right), \tag{24}$$

where ω_k and ν_k are mutually independent Gaussian process and observation noises with $\sigma_w^2 = 10$ and $\sigma_\nu^2 = 1$. The initial state is taken to be $x_0 = 0.1$. Figure 3 displays the performance of three particle filtering strategies in estimation of the state and output variables. The time variation of the effective sample size during SIS filtering shows that severe degeneracy occurs during almost all time steps (when $N_{eff} < N_p$). As noted earlier, degeneracy occurs when most of the particles have negligible weight, so that the variance of importance weights increases over time and the particles lose their ability to correctly approximate the posterior distribution. If resampling is performed when the effective sample size becomes less than a specified threshold (here 700 particles), then the effective sample size generally increases, resulting in improvement of accuracy; lower root-mean-square error (RMSE) is achieved for both state estimation and prediction, with more realistic uncertainty bounds. However, SIR (which resamples at every time step) eliminates the degeneracy problem completely with the effective sample size remaining almost equal to the total sample size, resulting in significant improvements to the approximations of estimation and uncertainty bounds. Figure 3 shows the RMSE of the posterior mean and true values in both state-space and the prediction for the different filtering strategies. Considering the superior performance of the SIR algorithm, we have adopted this procedure and demonstrate the extension of its applicability to parameter and state uncertainty estimation for hydrologic models.

3.5. SIR Particle Filtering in State-Parameter Space

[22] Considering that the main purpose of this study is to implement particle filtering for joint state-parameter esti-

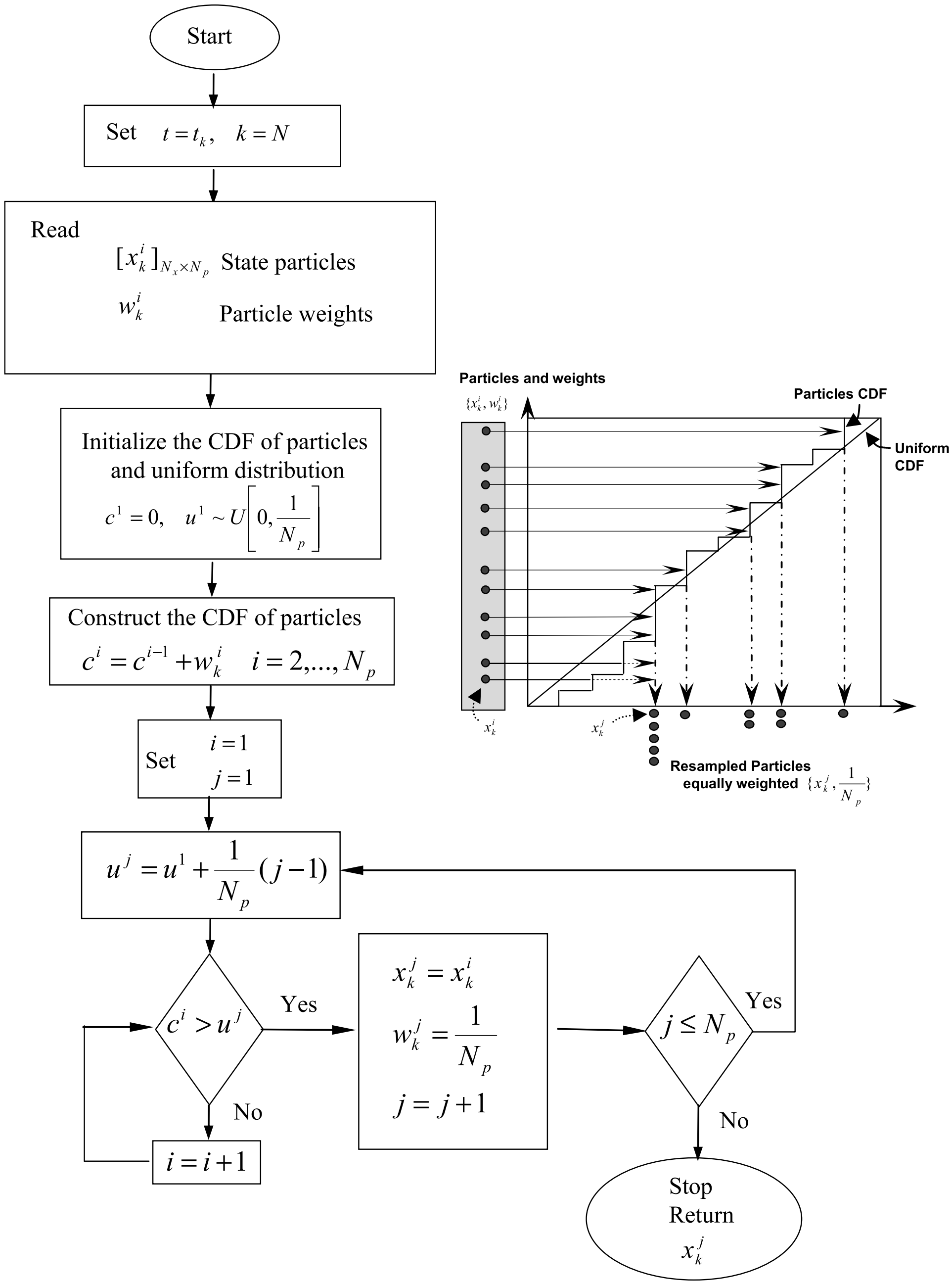

Figure 2. Resampling procedure flowchart and an example of the resampling process. A random particle x_k^i with weight w_k^i is mapped into a new indexed particle x_k^j with weight $1/N_p$. See color version of this figure in the HTML.

mation and uncertainty assessment, in addition to resampling of the state variables, resampling in the parameter space is also carried out using a proposal density of the form

$$q(\theta_{k+1} | \theta_k, y_{k+1}) = p(\theta_{k+1} | \theta_k). \tag{25}$$

[23] Although the effects of degeneracy can be reduced through resampling, a problem known as sample impoverishment leads to many particles having high weights w_k^i being selected many times, leading to a loss of diversity among particles. *Gordon et al.* [1993] illustrated that this problem becomes apparent when the dynamical system is noise-free or has a very small noise causing the particles to lack the opportunity to move in space stochastically. Therefore the process noise in the forward equation (1) plays a major role in particle filter performance by reducing the tendency toward sample impoverishment. In the case of parameter estimation, with the absence of an explicit form for the forward equation we can avoid parameter sample impoverishment by perturbing the resampled parameters (see the resampling procedure outlined in Figure 2) to be used at each successive time step:

$$\theta_{k+1}^i = \theta_{k-resamp}^i + \varepsilon_k^i \qquad \varepsilon_k^i \sim N\left(0, s^2 Var_k^\theta\right), \tag{26}$$

where ε_k^i is a small random noise, normally distributed with zero mean and variance $s^2 Var_k^\theta$. Var_k^θ is the variance of

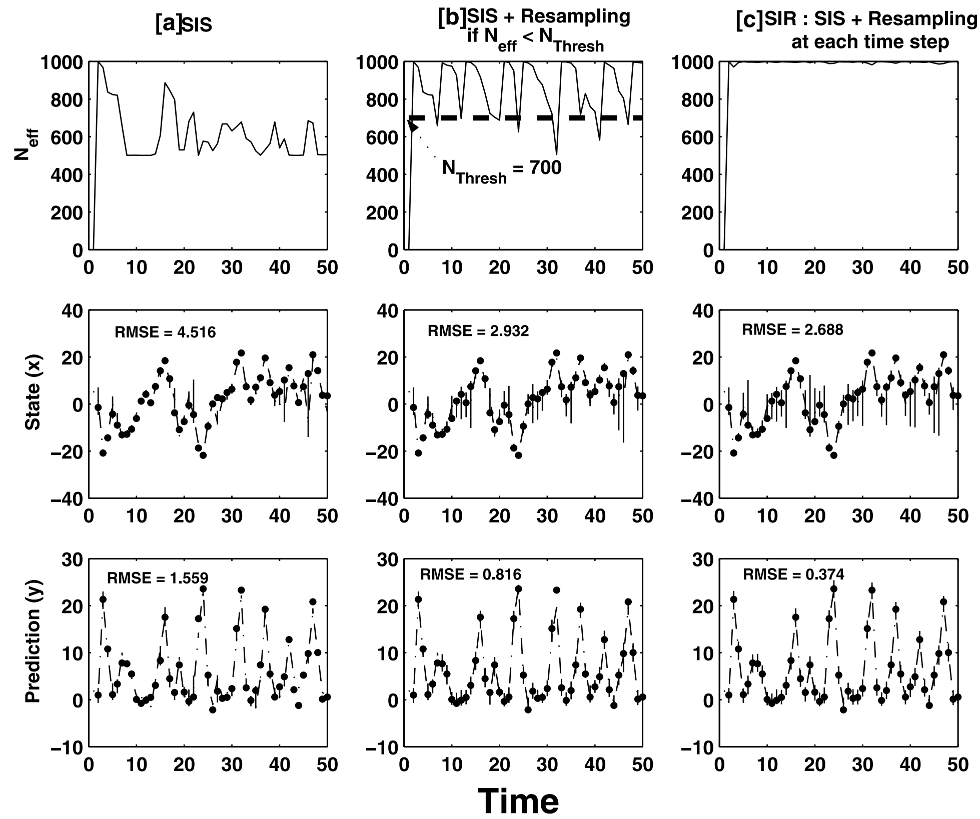

Figure 3. Sequential Monte Carlo analysis for state estimation and prediction in a one-dimensional state-space model using 1000 particles. (a) Sequential importance sampling (SIS). It is seen that degeneracy occurs at almost all time steps. (b) SIS + resampling when the effective sample size becomes less than the threshold (700 particles). (c) Sampling importance resampling (SIR): SIS + resampling at each time step. Solid circles and dash-dotted lines in state and prediction subplots denote the true value and the estimate, respectively; vertical solid lines represent the uncertainty bounds associated with the 95% confidence interval. See color version of this figure in the HTML.

parameter particles at time k before resampling, and s is a small tuning parameter which determines the radius around each particle being explored. This representation of SIR particle filtering generates model parameter ensembles via resampling to avoid degeneracy and parameter perturbation to avoid sample impoverishment. A full description of the SIR algorithm in a joint state-parameter space is given below and illustrated in Figure 4.

[24] 1. Model state initialization: Initialize N_x −dimensional model state variables for N_p particles, x_k^i, $i = 1,\ldots, N_p$, $x \in \Re^{N_x}$.

[25] 2. Parameter sampling: Sample N_θ −dimensional model parameters for N_p particles

$$\theta_k^i, i = 1, \ldots, N_p, \qquad \theta \in \Re^{N_\theta}.$$

[26] 3. Particle weight assignment: Assign the particle weights uniformly,

$$w_k^i = \frac{1}{N_p} \qquad i = 1, \ldots, N_p.$$

[27] 4. Model state forecast step: Propagate the N_p state variables and model parameters forward in time using the nonlinear model operator $f()$,

$$x_{k+1}^i = f\left(x_k^i, \theta_k^i, I_k\right) + \omega_{k+1} \quad \omega_{k+1} \sim N(0, Q_{k+1}).$$

[28] 5. Observation simulation: Use the observation operator $h()$ to propagate the model state forecast,

$$y_{k+1}^i = h\left(x_{k+1}^i, \theta_k^i\right) + \nu_{k+1} \qquad \nu_{k+1} \sim N(0, R_{k+1}).$$

[29] 6. Estimate the likelihood:

$$L\left(y_{k+1}|x_{k+1}^i, \theta_k^i\right) = \frac{1}{(2\pi)^{1/2}|R_{k+1}|^{1/2}} \times \exp\left(-\frac{1}{2R_{k+1}}\left[y_{k+1} - h_{k+1}^i(.)\right]^2\right)$$

$$p\left(y_{k+1}|x_{k+1}^i, \theta_k^i\right) = \frac{L\left(y_{k+1}|x_{k+1}^i, \theta_k^i\right)}{\sum_{i=1}^{N_p} L\left(y_{k+1}|x_{k+1}^i, \theta_k^i\right)} = p\left[y_{k+1} - h_{k+1}^i(.)|R_{k+1}\right].$$

[30] 7. Obtain the updated particle weight (filtering posterior):

$$w_{k+1}^i = \frac{w_k^i \cdot p\left[y_{k+1} - h_{k+1}^i(.)|R_{k+1}\right]}{\sum_{i=1}^{N_p} w_k^i \cdot p\left[y_{k+1} - h_{k+1}^i(.)|R_{k+1}\right]}.$$

[31] 8. Resampling: Apply the resampling procedure flowchart outlined in Figure 2 for all states and parameters, and store the resulting particles as $\theta_{k-resamp}^i$, $x_{k-resamp}^i$.

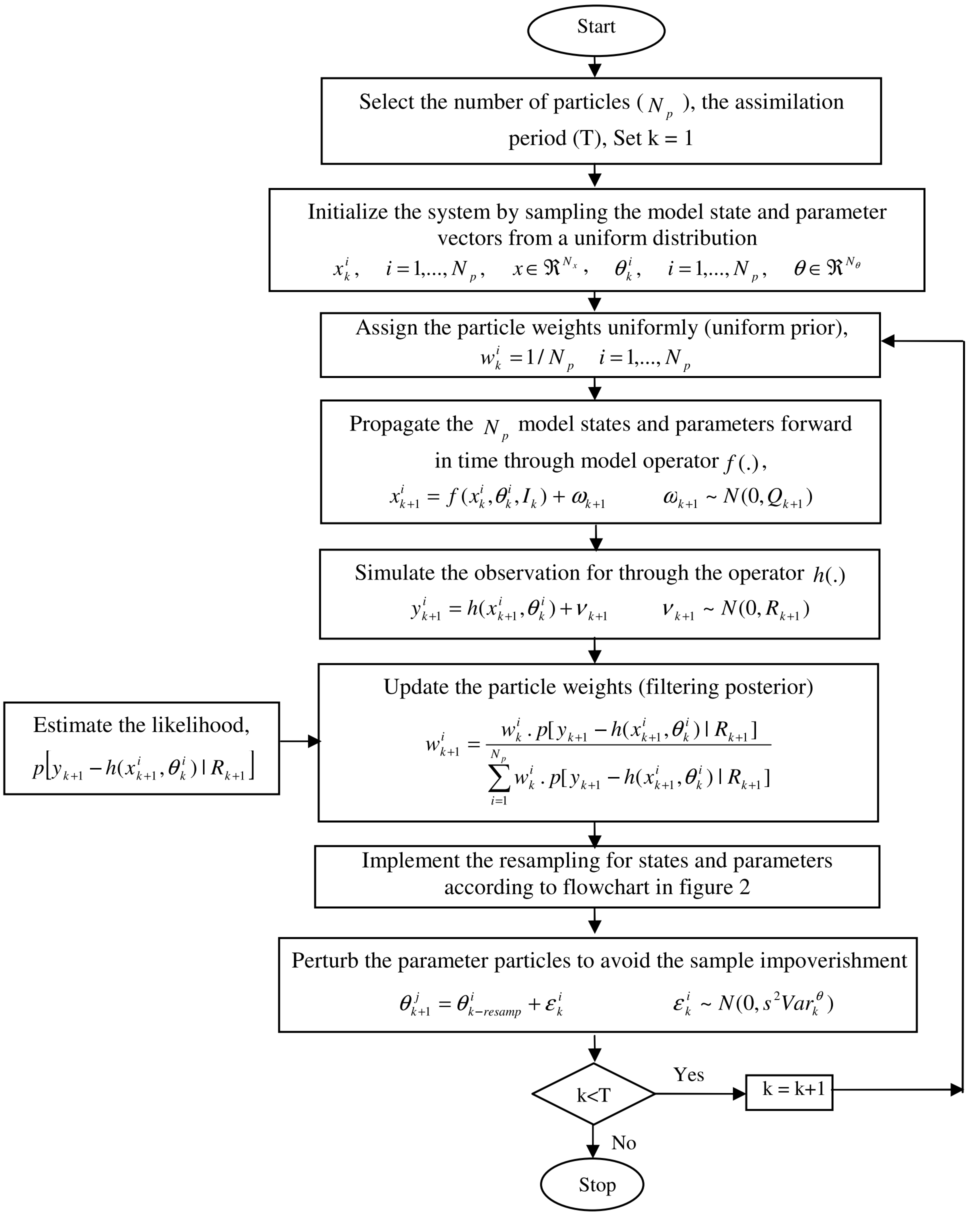

Figure 4. SIR particle filtering flowchart for estimating the posterior distribution of parameters.

[32] 9. Parameter particle perturbation: Perturb the particles within a small neighborhood to avoid sample impoverishment

$$\theta_{k+1}^i = \theta_{k-resamp}^i + \varepsilon_k^i \qquad \varepsilon_k^i \sim N\left(0, s^2 Var_k^\theta\right).$$

[33] 10. Check the stopping criterion: If k is equal to the desired number of time steps, stop; otherwise $k = k + 1$ and return to step 3.

4. Case Studies

[34] We present two case studies using a parsimonious conceptual watershed model to demonstrate the capability and usefulness of the SIR particle filter for estimating the parameters, state variables, and prediction uncertainties. The first synthetic case study is used to illustrate the power of particle filter for tracking the uncertainty bound associated with parameters and state variables where synthetic "observations" of streamflow are assimilated into the model. The second case investigates the applicability of the same filter for recursive parameter uncertainty estimation by assimilating historical observations of streamflow. We conclude by discussing the necessity for considering other sources of uncertainties to attain more accurate model predictions.

[35] The simple conceptual hydrologic model (HyMOD) has its origins in the probability distributed moisture model (PDM) [*Moore*, 1985] and has been used by several authors for testing batch and recursive calibration strategies [*Boyle et al.*, 2000; *Wagener et al.*, 2001; *Vrugt et al.*, 2003; *Misirli et al.*, 2003; *Moradkhani et al.*, 2005]. HyMOD is an extension of simple lumped storage models developed in the 1960s and consists of a nonlinear rainfall excess model (see *Moore* [1985, 1999] for details) connected in series with an arrangement of linear routing reservoirs (three identical quick-flow tanks in parallel with a slow-flow tank

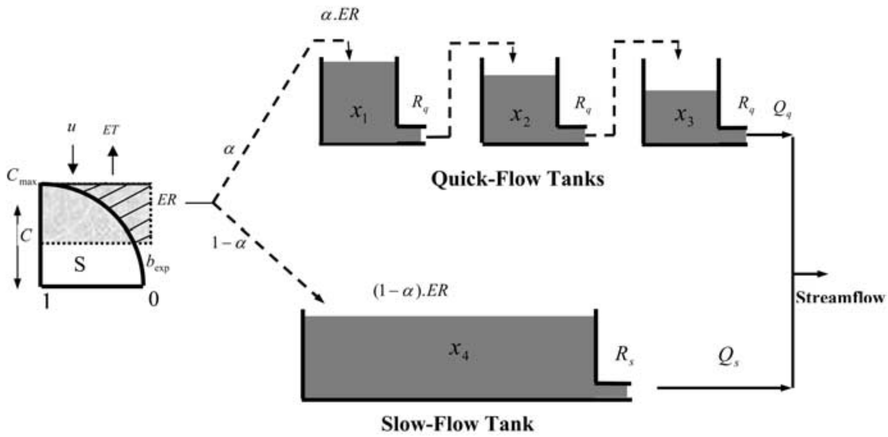

Figure 5. Schematic of the conceptual hydrologic model (HyMOD). See color version of this figure in the HTML.

Table 1. Prior Uncertainty Range Associated With Parameters in HyMOD

Parameter	Description	Minimum	Maximum	True Values
R_q	residence time for quick-flow tanks	0.00	0.99	0.46
R_s	residence time for slow-flow tank	0.001	0.10	0.03
α	partitioning factor between tanks	0.60	0.99	0.83
b_{exp}	spatial variability of soil moisture capacity	0.00	2.00	0.38
C_{max}	maximum storage capacity of watershed	0.00	1000	350

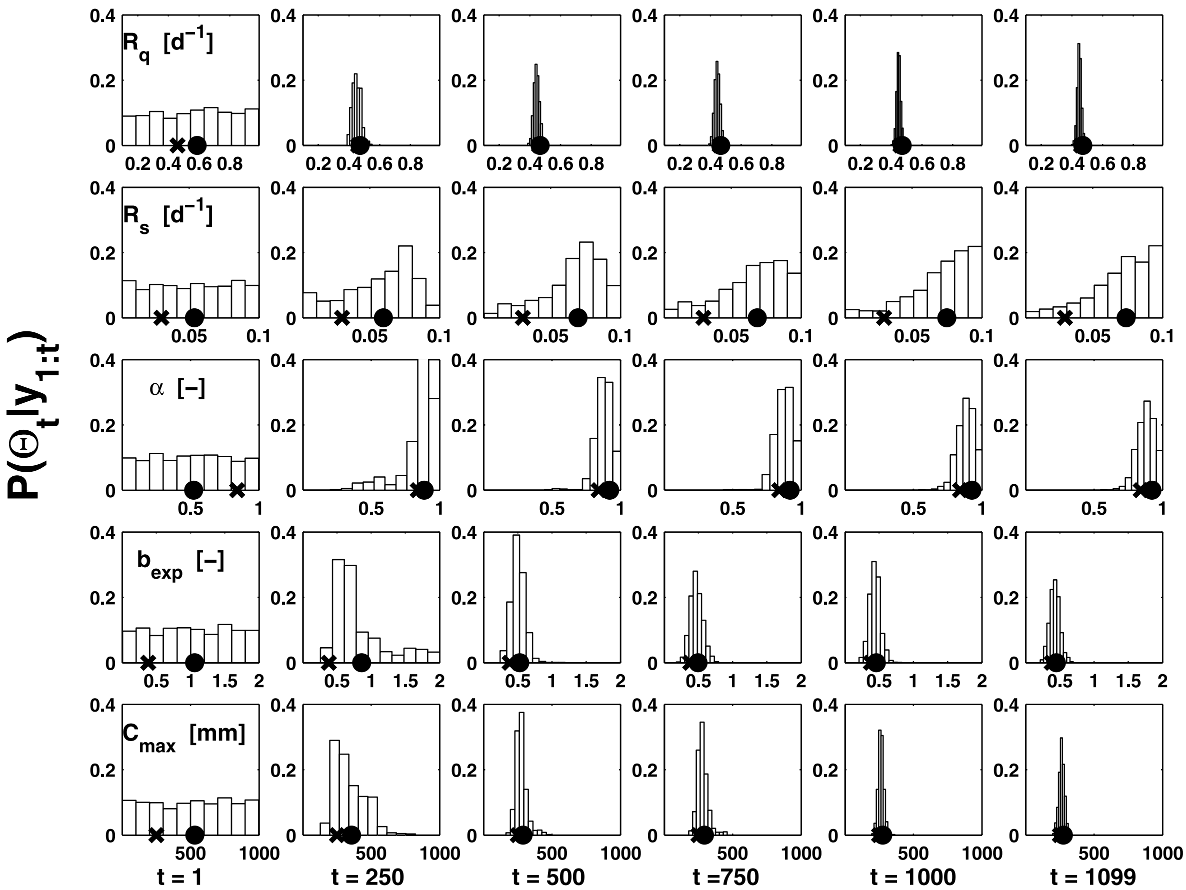

Figure 6. Time evolution of the HyMOD posterior parameter distributions at six different time segments by assimilation of synthetic streamflow. The crosses and solid circles denote the true and expected values, respectively, for each parameter.

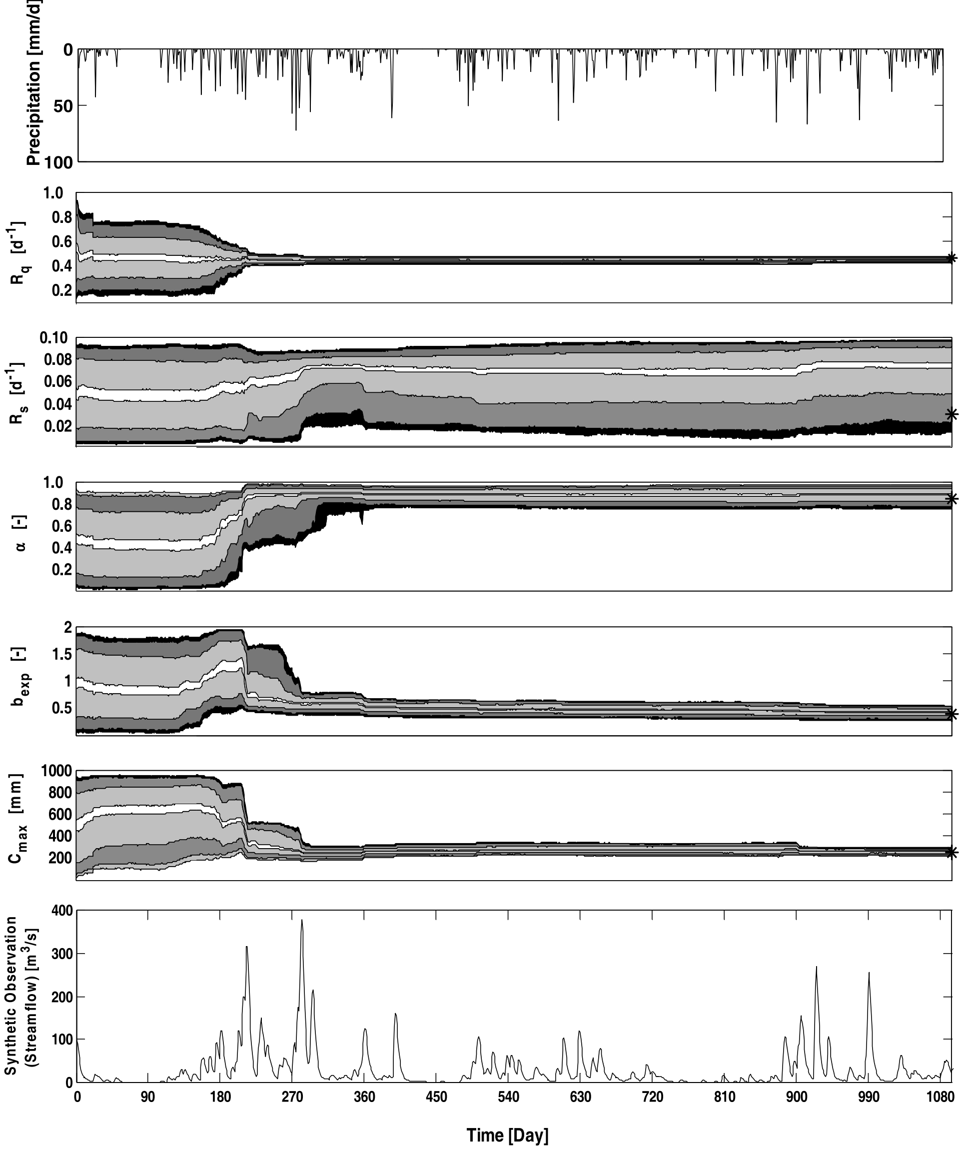

Figure 7. Uncertainty bound evolution of the parameters in the HyMOD for 3 years assimilation of synthetic streamflow. Shaded areas correspond to 95, 90, 68, and 10 percentile confidence intervals. Asterisks at end of each parameter subplot represents the true parameter values. See color version of this figure in the HTML.

representing the groundwater flow) (see Figure 5). The state variables in this system are S (the storage in the nonlinear tank representing the watershed soil moisture content, x_1, x_2 and x_3), the quick-flow tank storages representing the temporary (short-time) detentions (e.g., depression storages), and x_4, the slow-flow tank storage (subsurface storage). The model assumes that the spatial variation of soil moisture storage capacity across the watershed can be described by the function

$$S_t = S_{\max}\left[1 - \left(1 - \frac{c}{c_{\max}}\right)^{b_{\exp}+1}\right] 0 \le c \le c_{\max}, \qquad (27)$$

where $S_{\max}$ and $c_{\max}$ are related by

$$S_{\max} = \frac{c_{\max}}{b_{\exp} + 1}. \qquad (28)$$

[36] The model has five parameters that must be specified from knowledge of the real system or estimated using input-output observational data: $C_{\max}[L]$, the maximum storage capacity within the watershed; $b_{\exp}[-]$, the degree of spatial variability of the soil moisture capacity within the watershed; $\alpha[-]$, partitioning factor of the flow between quick-flow and slow-flow tanks; and $R_q[T]$ and $R_s[T]$, the residence times of the linear tanks, respectively.

[37] For the synthetic case study we assimilate synthetic streamflow "observations" generated via a free run of the model using a predefined set of "true" parameters and assuming that the forcing data (input) are noise free. In this setting the model structure is considered to be perfect, and therefore the only source of uncertainty is associated with the parameter estimates. To make the estimation problem insensitive to specification of the initial condition, an ensemble of 1000 uniformly distributed values for the initial

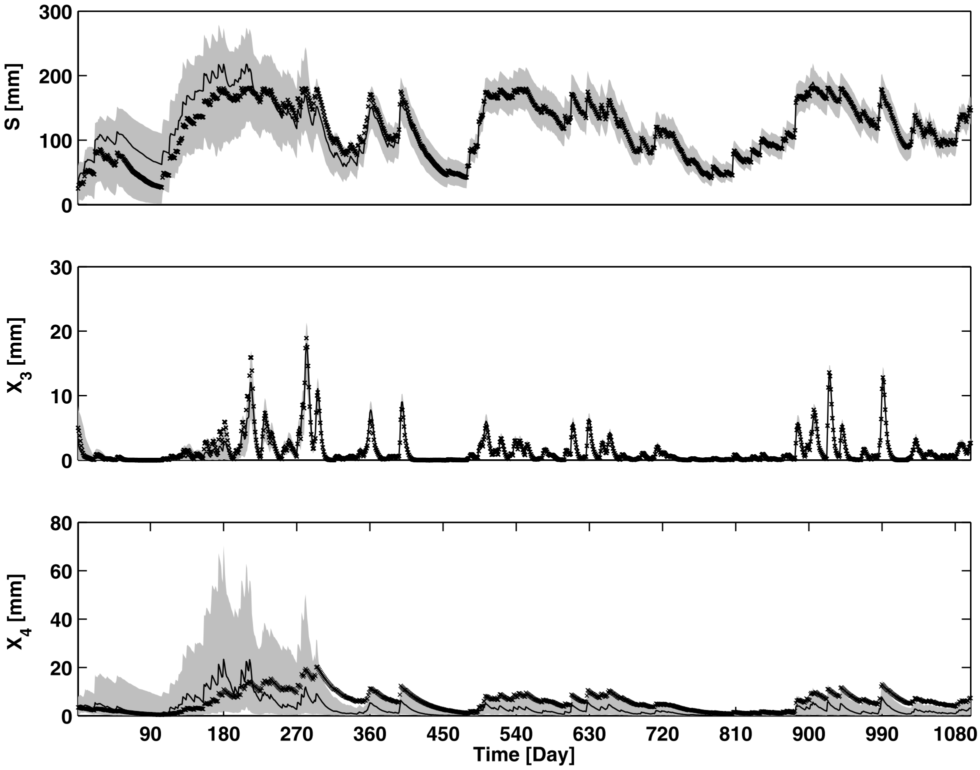

Figure 8. Uncertainty bound tracking of three state variables in the HyMOD. (a) Storage in the nonlinear tank which is conceptually functioning as watershed soil moisture. (c) Quick flow tank storage. (c) Slow-flow tank storage. Shaded areas correspond to 95% uncertainty bounds, and crosses and solid lines denote the synthetic and expected values. See color version of this figure in the HTML.

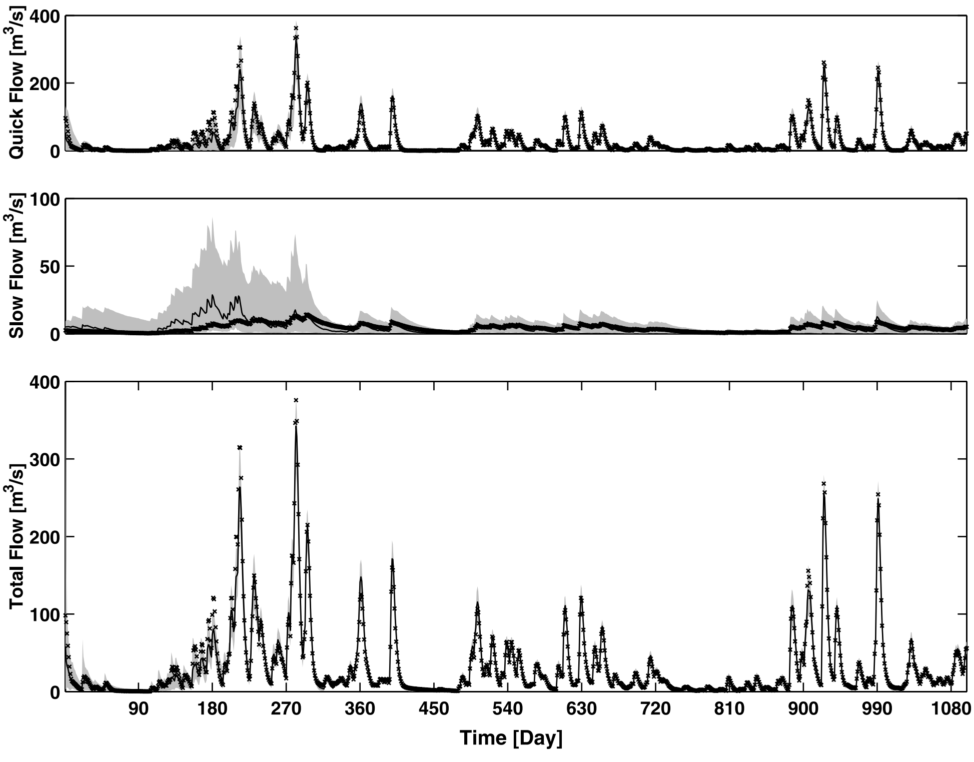

Figure 9. Results of the SIR particle filter for hydrograph prediction using the HyMOD conceptual watershed model by assimilating synthetic streamflow. (a) Quick flow from the third quick-flow tank. (b) Slow flow from the slow-flow tank. (c) Total streamflow as the summation of quick flow and slow flow. Shaded areas in all subplots correspond to 95% confidence intervals in prediction. Crosses and solid lines denote the synthetic and expected values of streamflow, respectively. See color version of this figure in the HTML.

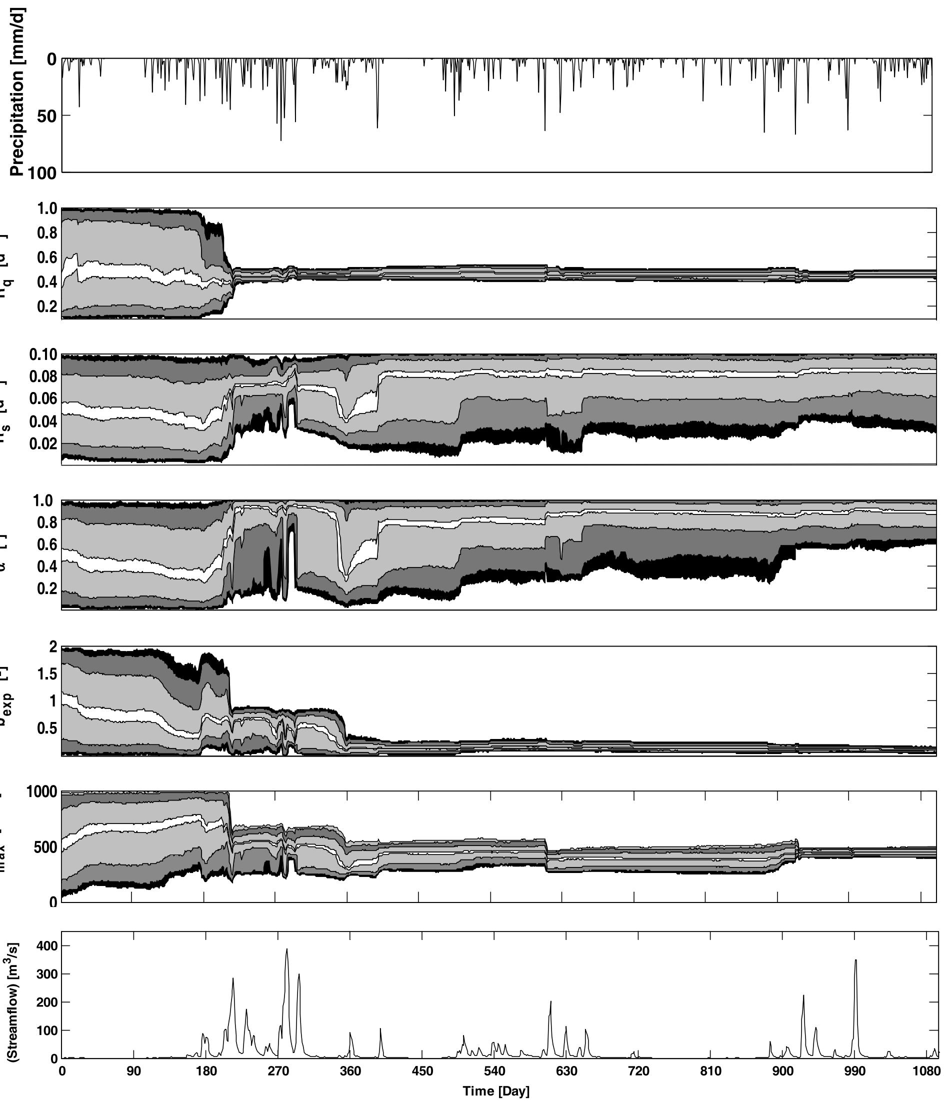

Figure 10. Uncertainty bound tracking of parameters in the HyMOD conceptual watershed model for 3 years assimilation of historical streamflow of the Leaf River watershed for the period 28 July 1952 to 28 July 1955. Shaded areas correspond to 95, 90, 68, and 10 percentile confidence intervals. See color version of this figure in the HTML.

state variables is generated. The prior estimates of the parameter uncertainty is made by guessing at a wide but plausible range of values for the parameters. The prior range and true values (synthetic true) are shown in Table 1. Hence the parameter particles are sampled within the predefined range using a uniform distribution. SIR filtering in the parameter space was carried out at each time step and posterior probability density estimated as illustrated in Figure 6 for six time segments; notice that as the assimilation proceeds, the posterior mean estimates for all the parameters are converging toward the observation. The uncertainty bounds on the residence time parameter for the slow-flow tank are the slowest to narrow, in comparison with the other parameters (see also Figure 7, where the time evolution of uncertainty bounds with 95, 90, 68, and 10 percentile confidence is displayed). As seen from precipitation and streamflow subplots in Figure 7, the beginning of the time series reveals the low-flow period which obviously does not significantly help lead parameter samples to the right region. In other words, information content in the beginning of time series is not enough to identify the parameters properly. Since a recursive strategy is used in this study, the method relies on the information content in the new data. This is reflected by the likelihood and prior which are changing by availability of new information. A significant reduction of uncertainty after about 200 days is observed for four of the parameters. The reason for these reductions can be attributed to the key role of observation (here synthetic streamflow) in updating (correcting) of parameter samples. The ensembles of four parameters which are moving toward the right region (true values) in parameter space begin to be influenced partially by moderate event (time step 180) and to higher extent by major event (time step 200). This is in agreement with the findings of *Vrugt et al.* [2002] and *Wagener et al.* [2003]. In regards with the identifiability of parameters, the findings in this study are

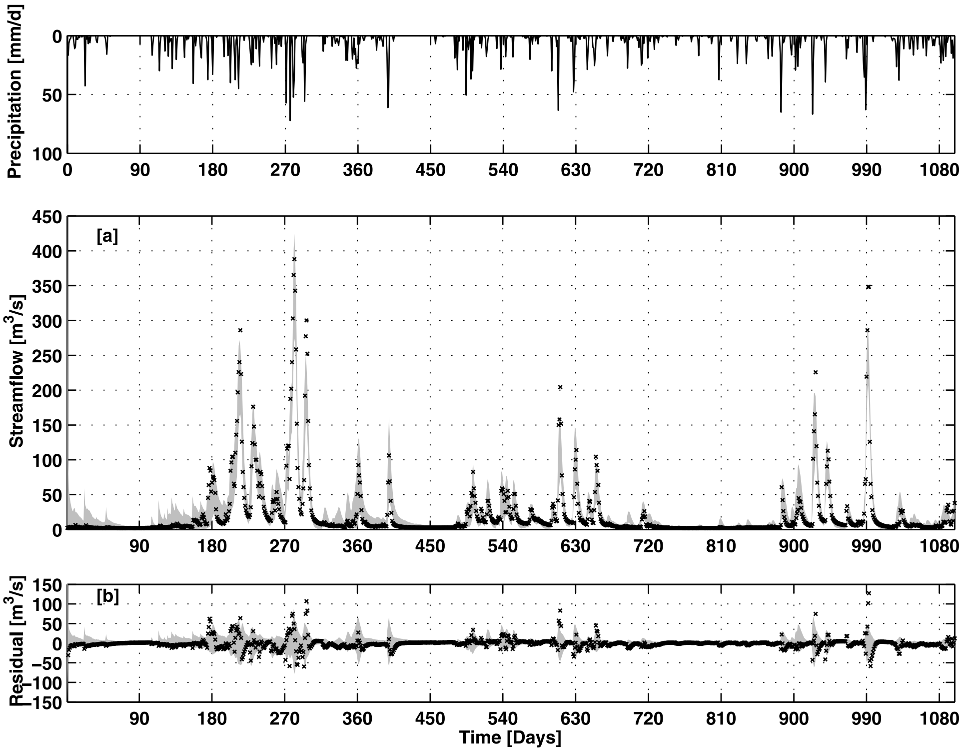

Figure 11. Result of the SIR particle filter for hydrograph prediction using the HyMOD by assimilating historical streamflow of the Leaf River watershed for the period 28 July 1952 to 28 July 1955. (a) Hydrograph uncertainty bounds with 95% confidence interval associated with the derived posterior parameter distribution using 1000 particles. (b) Residual bounds associated with 95% confidence interval and observations (streamflow). See color version of this figure in the HTML.

different from those two studies presumably due to (1) the difference in time series used, especially that in the current study the time evolution of predictive uncertainties is influenced by information content through available data, and (2) the mutual interaction considered between state variables and parameters. Therefore the behavior of parameters is influenced by state variables as well (Figure 8). It was found that slow-flow parameter R_s is less identifiable, unlike other parameters that converge to the true values in less than a year. However, the combinatorial effect of parameter-state values results in a satisfying result as depicted in Figure 9. The slow convergence of the uncertainty bounds for the slow-flow tank parameter R_s can be explained by its minimal contribution to the volume of streamflow. Figure 8 allows comparison of the time evolution of the uncertainty bounds for three of the state variables (nonlinear tank storage S, last quick-flow tank storage x_3, and slow-flow tank storage x_4). At the early stage of filtering, the uncertainty is high for nonlinear and slow-flow tank storages. Because the quick-flow tank is most strongly correlated with the observations (streamflow), it is most easily and quickly identifiable. However, the streamflow prediction via the observation equation (2) results from the combined effect of the highly interactive state and parameter values, complicating the assimilation of the streamflow measurement into the quick-flow and slow-flow components (Figure 9). Because the quick flow is highly correlated with the observation, it rapidly achieves a smaller uncertainty bound while the uncertainty in the slow flow diminishes slowly. Note that for purposes of clarity the plots have been displayed in different scales and that the uncertainty associated with the slow flow in the normal scale is actually almost negligible, despite the high uncertainty in slow-flow parameter and storage. The case studies shows that the procedure is able to identify even the less influential components in generating the predictive variable (here streamflow) of the highly interactive (state-parameter) system.

[38] We next implement the methodology to a real case study by assimilating the historical streamflow into the model. Filter performance was tested using 3 years of data (28 July 1952 to 28 July 1955) from the 1944-km^2 Leaf River watershed, located north of Collins, Mississippi. The data, obtained from the National Weather Service Hydrology Laboratory, consist of mean areal precipitation (mm/d), potential evapotranspiration (mm/d), and streamflow (cm^3/s).

[39] The system setup, including the prior uncertainty range for the parameters and number of particles in state and parameter space, remains as before. The time evolution of uncertainty bounds for different confidence intervals is displayed in Figure 10. Parameters R_q, $b_{\exp}$, and $C_{\max}$ are seen to converge to specific regions of the parameter space with relatively small uncertainty bounds in comparison with parameters α and R_s. Figure 11 presents the prediction uncertainty ranges for the HyMOD simulated streamflow corresponding to SIR particle filter. Despite generally good conformity between observed and

simulated time series, some of the high-flow events do not lie within the prediction uncertainty bounds. This indicates that the attribution of the uncertainty to only the parameter estimates is inappropriate. In continuing studies, the roles of various other sources of uncertainties including those attributable to the model structure, forcing data observation (precipitation), and output observation (streamflow) must also be considered.

5. Summary and Conclusion

[40] We have investigated the use of a sequential Monte Carlo method, also known as a particle filter, for practical uncertainty assessment of parameter and state estimation in a conceptual hydrologic model. Although the Kalman filter is highly effective and efficient if the underlying assumptions hold, it is limited by its closure at the second-order moments (i.e., the filter evolution is controlled by its second-order characteristics and Gaussian distribution of error components). In real hydrologic applications, the assumptions of system linearity or Gaussian error model do not hold. Nonlinear Bayesian parameter estimation methods such as BaRE do not treat the joint state-parameter uncertainty, while also suffering from a tendency toward sample degeneracy caused by the inability to properly sample the evolving conditional posterior parameter density. Recent developments in sequential Bayesian estimation based on Monte Carlo methods make the application of improved techniques possible for more accurate uncertainty assessment of hydrologic models. Particle filters are able to handle model nonlinearities while computing a complete (arbitrarily accurate) representation of the posterior distribution so that any statistical measure of the quantities of estimate can easily be computed. In this paper we discussed the use of particle filters for state-parameter uncertainty estimation using sequential importance sampling (SIS) and sampling importance resampling (SIR). The SIR particle filter was extended to handle estimation of the joint parameter and state posterior distribution. To avoid sample impoverishment, a small random perturbation was applied to the parameter samples after resampling. A synthetic case study was used to test the power and applicability of the methodology using a simple but representative conceptual watershed model (HyMOD). A further application using actual observations of historical streamflow data from Leaf River watershed showed that despite good agreement between the observed time series and the simulated predictions, some of the high flows fall outside of the estimated prediction uncertainty intervals. This supports the findings of other studies [e.g., *Thiemann et al.*, 2001; *Wagener et al.*, 2003; *Gupta et al.*, 2003a; *Vrugt et al.*, 2003; *Moradkhani et al.*, 2005] that the role of other sources of uncertainty (e.g., model structural error and input measurement errors) must also be considered to improve accuracy in the model predictions. Research aimed at further improvements to the current filtering algorithm, including the resampling procedure and methods for accounting for various sources of uncertainties, will continue and be reported in the future. Methods for improving the computational efficiency of the particle filter for larger systems are also an open area for further research.

[41] We close by noting that particle filters are easily and directly applicable to more complex models such as land surface models where the estimation of state posterior distributions is of major concern. However, successful data assimilation relies on unbiased prediction of the model state, which is largely dependent on accurate model parameterization. For model parameters that cannot be determined directly by measurement, the particle filter provides an attractive approach for joint estimation of parameter uncertainty in addition to the model state uncertainty. Nonetheless, prospective improvement in sequential Monte Carlo (particle filtering) applicable to any hydrolometeorological model is an open issue and we welcome the exchange of ideas related to it. The software used for the current work is available by request from the first author.

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