Convergence of approaches toward reducing uncertainty in predictions in ungauged basins

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[1] The focus in the search for more reliable predictions in ungauged basins (PUB) has generally been on reducing uncertainty in watershed models (mainly their parameters). More recently, however, we seem to remember that the ultimate objective is not to define the parameters of a specific model but to understand the watershed: What behavior do we expect the ungauged watershed to exhibit? And what behavior should not occur in a particular ungauged watershed? The answers to these questions actually provide additional information that can be assimilated in watershed models for uncertainty reduction in PUB. This extension to hydrologic modeling approaches provides a quantitative link between watershed modeling and statistical hydrology as well as process hydrology that has to be explored. We witness a convergence of approaches—Bayesian, set theoretic, and optimization based—toward utilizing this link. The result is an opportunity for the (quantitative) dialog between modelers, statistical hydrologists, and experimentalists. We close our discussion of this development by presenting new and exciting research questions that we now have to address.

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1. Introduction

[2] Current watershed models rely on rainfall-runoff observations to learn during a calibration process how a particular watershed functions so that a model can reproduce observed patterns. This calibration process is necessary since reliable reproduction of observed hydrologic system behavior by the model is often unobtainable from the physical watershed characteristics alone. This is partially due to our inability to observe all aspects of the system in sufficient detail, e.g., geology, but also due to the problem of translating such information (if it was available) into actual model parameters at scales different from the measurement. The lack of streamflow observations in the vast majority of catchments of the world and the uncertainty associated with model predictions at these locations are seen as major limitations for hydrological science today [*Sivapalan*, 2003]. In particular, the absence of gauges in many small streams demands research into better modeling tools for streamflow simulations in different hydroclimatic and geologic settings [*National Research Council* (*NRC*), 2004]. Figure 1 provides an example which shows that in the United States stream length is dominated by small streams, while gauges are biased toward large streams [*Poff et al.*, 2006; *Nadeau and Rains*, 2007].

[3] Consequently, there are urgent calls from the hydrological, ecological, and water resources communities to improve the credibility of hydrological predictions across environmental systems [*Sivapalan et al.*, 2003; *NRC*, 2004; *Poff et al.*, 2010; *Palmer*, 2010]. *Vogel* [2006, p. 63] even concluded that "Given the increasingly widespread usage of watershed models for solving environmental problems, the regionalization of watershed models may be one of the most challenging and fundamental problems within the entire field of hydrology." Despite these needs, existing monitoring networks continue to decline because of financial and man power limitations [*Stokstad*, 1999]. This situation is of particular concern for those regions of the world where resources for hazard mitigation and adaptation are extremely poor and hence vulnerability is high [*Kapangaziwiri and Hughes*, 2008]. There has therefore been a concerted effort by the international hydrological community through the International Association of Hydrological Sciences Predictions in Ungauged Basins initiative to reduce the uncertainty in hydrologic predictions in ungauged basins (PUB) [*Sivapalan et al.*, 2003; *Montanari*, 2011].

[4] In this commentary, we define the issue of uncertainty in PUB, discuss traditional and recent approaches for uncertainty reduction, point out the convergence of methods that is emerging, and, finally, list open research questions that demand an answer.

2. Uncertainty in Hydrological Modeling for PUB

[5] The issue of uncertainty in hydrological modeling has been widely discussed. It is not the intention of this opinion paper to repeat or even to review this discussion, nor is it necessary for the point we are trying to make. *Liu and Gupta* [2007] recently reviewed the topic of uncertainty in hydrological modeling, framing it in the context of data assimilation, and we refer the reader to their paper for much greater detail than is provided here. A wide range of sources contribute uncertainty to hydrological predictions [*Liu and Gupta*,

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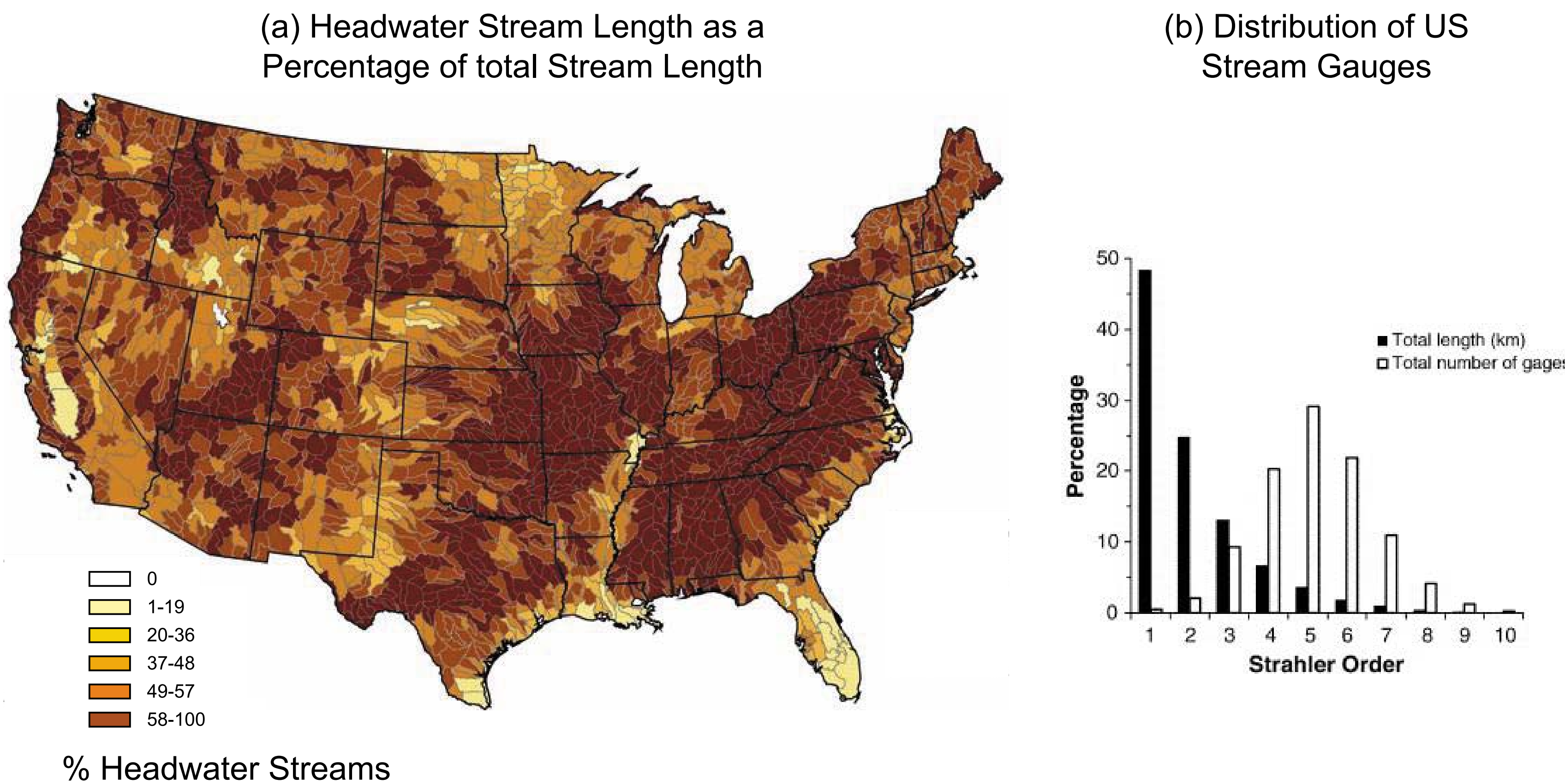

Figure 1. (a) Spatial distribution of headwater stream length as a percentage of total stream length [from *Nadeau and Rains*, 2007]. (b) Distributions of stream length and stream gauges against stream order (reprinted from *Poff et al.* [2006], with permission from Elsevier).

2007; *Montanari et al.*, 2009; *Beven*, 2008; *Montanari*, 2011], including observations [*Kavetski et al.*, 2006a, 2006b; *Di Baldassarre and Montanari*, 2009; *Younger et al.*, 2009; *Liu et al.*, 2009; *McMillan et al.*, 2010], the model structure and its parameters [*Beven and Binley*, 1992; *Kuczera and Parent*, 1998; *Vrugt et al.*, 2003; *Butts et al.*, 2004; *Marshall et al.*, 2007; *Ajami et al.*, 2007; *Clark et al.*, 2008], and initial conditions [*Koutsoyiannis*, 2010]. While we acknowledge the need to better understand the impact of observational error and other error sources, we focus here on the possibility of reducing uncertainty in situations where observations of the system response behavior of interest, most often streamflow, are unavailable.

[6] In a typical modeling process one will start by selecting one or more model structures, M, to represent the system at hand [see *Liu and Gupta*, 2007]. For a gauged basin, the modeler would then test how well the model or each model reproduces the observed system response, z, by visual comparison of observations and simulations or by explicitly calculating some goodness of fit measures. Most often, however, a single model structure is selected from the start, and the focus shifts toward reducing the uncertainty in the model parameters, θ. The modeler will implicitly or explicitly define a prior probability, $p_{\text{prior}}(\theta)$, of how well the system might be represented by a given parameter set, most often on the basis of his or her experience with a particular model at similar locations. Then the defined parameter space can be explored, and for each candidate parameter set θ a likelihood function, $L(\theta|z)$, for the given observations z can be computed. The likelihood is proportional to the probability, $p(z|\theta)$, that the observations could have been generated by the parameter set θ. The likelihood function therefore defines how the observations z modify our prior knowledge of the parameter set, and by combining prior knowledge and likelihood using Bayes theorem, we can calculate the posterior probability for θ, $p_{\text{posterior}}(\theta|z)$ [e.g. *Box and Tiao*, 1973, p. 10]

$$p_{\text{posterior}}(\theta|z) \propto L(\theta|z)p_{\text{prior}}(\theta). \tag{1}$$

However, by definition, observations of the system response, z, are unavailable in ungauged basins, and hence all the attention has generally been placed on defining the priors on model and parameters as well (narrowly) as possible, while different (often informal) approaches are then used to refine such prior information. However, it is not true that in the absence of streamflow observations no information regarding the expected behavior of the watershed under study is available.

[7] In the absence of local observations of the system response, z, other, transferred information can be used to reduce uncertainty beyond what is possible by defining priors on model parameters [*Yadav et al.*, 2007]. We will call this information about the dynamic behavior of the watershed a signature. The likelihood is then derived from our expected value of the signature at the ungauged location rather than from historical observations, and equation (2) (and equally equation (1)) changes to

$$p_{\text{posterior}}(\theta|s) \propto L(\theta|s)p_{\text{prior}}(\theta), \tag{2}$$

where $L(\theta|s)$ now is the likelihood of a particular parameter set given the expected (but not locally observed) signature [*Bulygina et al.*, 2009]. The likelihood is higher for model-parameter combinations that simulate signature values closer to our expectation. In sections 3 and 4 we will discuss possible origins of both priors and signature-based likelihoods. It is important to stress that such a signature-based calibration will, of course, be possible in gauged basins as well; that is, the signatures are then derived from actual local observations.

3. The Traditional Approach: Priors on the Model and Its Parameters

[8] The traditional approach to solving the PUB problem puts the emphasis on reducing the uncertainty in the a priori model used for making the predictions, i.e., by defining priors on models and parameters. The typical starting point is the selection of a model structure according to experience with the model, personal preference, or other criteria. We most often give the selected model structure a prior probability of 1 while neglecting other options [*Beven*, 2000]. Once a model structure is selected, the main focus shifts toward identifying appropriate parameters for the model in the absence of a sufficiently long record of observed streamflow observations that would enable traditional model calibration. Approaches to solving this parameter estimation problem (either as deterministic values or as prior distributions) generally follow one of three strategies: (1) the regionalization of the model parameters through calibration of the model to many watersheds and by deriving regression equations between parameters and watershed characteristics [e.g., *Sefton et al.*, 1995; *Post and Jakeman*, 1996; *Abdulla and Lettenmaier*, 1997; *Post et al.*, 1998; *Sefton and Howarth*, 1998; *Seibert*, 1999; *Fernandez et al.*, 2000; *Merz and Bloschl*, 2004; *Parajka et al.*, 2005; *Wagener and Wheater*, 2006; *Hundecha et al.*, 2008; *Oudin et al.*, 2008], (2) through a priori parameter estimates using only local physical characteristics of the watershed (e.g., soil hydraulic properties) [e.g., *Atkinson et al.*, 2002; *Koren et al.*, 2003; *Leavesley et al.*, 2003; *Yilmaz et al.*, 2008; *Kapangaziwiri and Hughes*, 2008; *van Werkhoven et al.*, 2009; *Hughes et al.*, 2010], and (3) the transfer of parameter sets (rather than individual parameters as in the first strategy) from donor watersheds on the basis of some measure of hydrological similarity between donor and transfer watershed [e.g., *McIntyre et al.*, 2005; *Buytaert and Beven*, 2009; *Reichl et al.*, 2009]. All three strategies have been shown to have strengths and weaknesses, and we do not want to repeat this discussion here. Ultimately, significant uncertainty remains in all three approaches because of watershed model structural error, lack of parameter identifiability during calibration, and a lack of reliable relationships between observable watershed characteristics and model parameters [e.g., *Wagener et al.*, 2004; *Wagener and Wheater*, 2006; *Bárdossy*, 2007]. While some uncertainty is likely to remain in any hydrologic predictions [e.g., *Koutsoyiannis*, 2010], further uncertainty reduction is clearly desirable in the PUB context.

4. Additional Information: Expected Watershed Behavior as Basis for a Likelihood or a Constraint

[9] The purpose of the calibration process in gauged basins is to extract information about the dynamic watershed behavior from long-term observations of streamflow (most often) or other hydrologic variables, therefore identifying parameters that reflect the functional characteristics of the system under study. Information extracted relates to func-

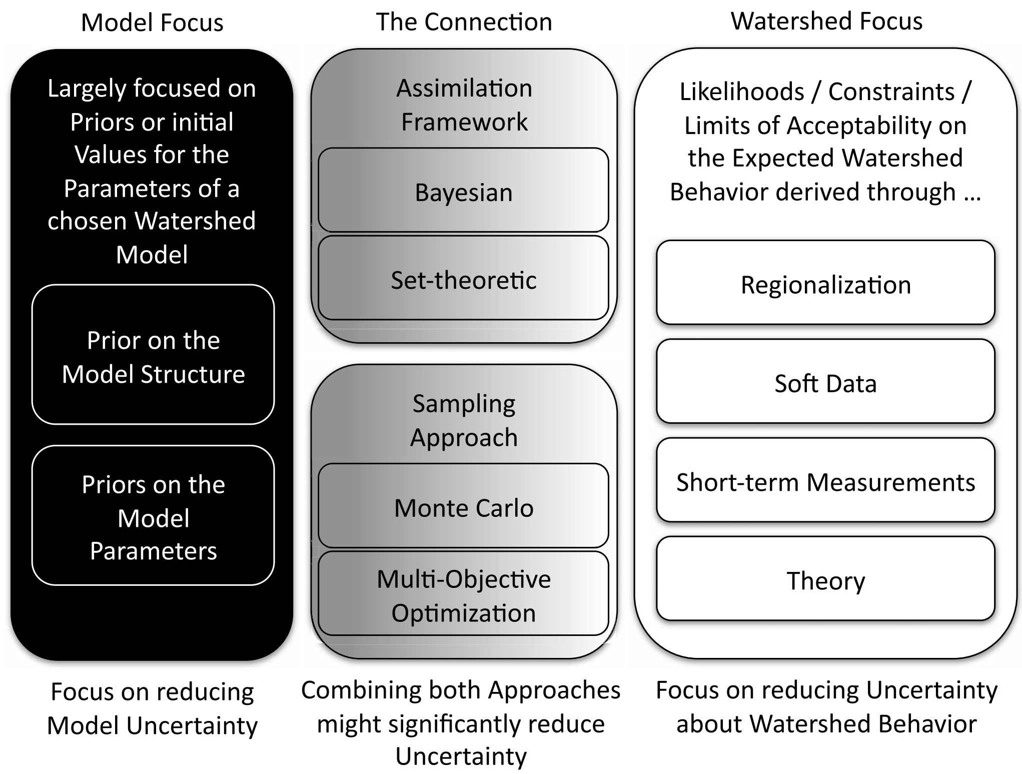

Figure 2. Schematic overview of both model- and watershed-focused approaches.

tional behavior such as the following questions: How much of the incoming precipitation will become evapotranspiration versus streamflow? How quickly does the hydrograph rise after a rainfall event starts? What is the shape of the streamflow recession after the rainfall stops?

[10] For ungauged basins we generally assume that none of this information is available beyond the knowledge that is embedded in the watershed model. However, this ignores other available sources of information. There are actually multiple ways in which we can derive additional information even without long-term local observations, and hence there should generally be some opportunity to condition a model even in the ungauged case, if this information can be quantified. That is, there is a way to define a likelihood that can be combined with the prior knowledge.

[11] We believe that the answer to this problem of utilizing more information is rapidly emerging across a range of recently published papers [*Spate et al.*, 2004; *Yadav et al.*, 2007, *Zhang et al.*, 2008; *Bulygina et al.*, 2009, 2011; *Winsemius et al.*, 2009; *Castiglioni et al.*, 2010; *Parada and Liang*, 2010; *Di Baldassarre et al.*, 2009; L. Lombardi et al., Calibration of a rainfall-runoff model at regional scale by optimising river discharge statistics: Performance analysis for different river flow regimes, submitted to *Physics and Chemistry of the Earth*, 2011]. The previous assumption of no information outside the model is increasingly challenged. The basic idea of all the papers listed above is to mimic the calibration process, though without the use of long-term or even any records of streamflow observations at the location of interest.

[12] All authors in the above listed studies attempt to derive additional (watershed model–independent) information about the expected dynamic watershed behavior at an ungauged location that can be assimilated into any watershed model. This information is (most often) provided in the form of hydrological signatures and/or streamflow indices that contain some information about the functional behavior of the watershed (for discussions on hydrological signatures see *Farmer et al.* [2003], *Wagener et al.* [2007], *Gupta et al.* [2008], and *Yilmaz et al.* [2008]). The challenge is to quantify the expected values of such signatures in the absence of historical streamflow observations. It is important to note that signatures can, of course, also relate to hydrological variables other than streamflow (e.g., groundwater or soil moisture). A basic assumption here is that these signatures contain (at least) some of the information about watershed function that is usually extracted during model calibration from historical streamflow data. Approaches to utilizing this additional information for PUB differ in how three main steps are implemented. The three steps are as follows (Figure 2): (1) quantification of the expected watershed dynamic behavior (i.e., what is the basis for estimating the signatures?), (2) the merger of this information with the previously defined priors (i.e., mainly whether distributions, ranges, or deterministic values are assimilated into the model and how this is done), and (3) the sampling of the model parameter (and potentially model structure) space to identify "behavioral" parameter sets (models) that produce simulated signatures consistent with the expected watershed behavior.

[13] A straightforward way to estimate probability distribution functions (PDFs) describing the expected behavior might be the regionalization of specific hydrologic signatures [*Castellarin et al.*, 2004; *Detenbeck et al.*, 2005; *Sanborn and Bledsoe*, 2006; *Pallard et al.*, 2009; *Brath et al.*, 2003; *Yadav*

et al., 2007], building on the long tradition of statistical hydrology, which has evolved very effective ways of transferring streamflow characteristics to ungauged locations [e.g., *Vicens et al.*, 1975; *Stedinger and Tasker*, 1985; *Lima and Lall*, 2010]. In this way one can combine local (catchment-scale) and regional behavior, therefore profiting from an increased amount of information, though not all information might be equally helpful to reduce predictive uncertainty [*Merz and Blöschl*, 2008a, 2008b]. In the ungauged case, different ways of incorporating regional information have been proposed. *Bárdossy* [2007] calibrated model parameters to regionalized signatures (means and variances of annual discharges) to improve PUB. *Yadav et al.* [2007] estimated regional regression equations for three signatures (base flow index, slope of the flow duration curve, and high pulse count), including the confidence and prediction limits on the regression equations. These limits provided constraints on feasible values for the three signatures at ungauged locations that were imposed on the ensemble predictions of a continuous watershed model. This strategy reduced PUB uncertainty by at least 50% by excluding all ensemble predictions that produced signatures outside the regionalized constraints while capturing over 80% of the observed streamflow. *Bulygina et al.* [2009] utilized the probability distribution derived from regionalizing base flow index using regression, therefore deriving not just behavioral and nonbehavioral parameter distributions as was done by *Yadav et al.* [2007] but actual PDFs. *Winsemius et al.* [2009] use a combination of hard (from actual data) and soft information to derive limits of acceptability [*Beven*, 2006] on three different streamflow signatures (shape of the recession curve, spectral properties of daily streamflow, and monthly water balance). *Castiglioni et al.* [2010] developed regional regression equations for the average value, standard deviation, and lag 1 autocorrelation coefficient of streamflow. Other statistical approaches to estimate flow characteristics have been proposed in recent years, such as top kriging or simple correlation, but so far they have not been combined with the use of continuous watershed models for PUB [e.g., *Skøien et al.*, 2006; *Skøien and Blöschl*, 2007; *Archfield and Vogel*, 2010].

[14] The ability to regionalize such signatures will, of course, have limits because of the uniqueness of watersheds [*Beven*, 2000, 2007]. There will certainly be outliers where watersheds respond very differently to the majority of systems and where generally available information about the physical characteristics of the watershed will be insufficient to identify them as outliers without observations of their hydrologic response. In particular, limited knowledge of geology often creates outliers since it is often a very strong influence on the hydrologic response [*Tague and Grant*, 2004].

[15] Other strategies focus more on using local information from the watershed under study. One example is the use of short-term measurement campaigns to estimate signatures, assuming that not all hydrologic characteristics require long-term observations of streamflow or other variables to be estimated. *Seibert and Beven* [2009], for example, show that short time series of streamflow or even single runoff measurements can be used for good parameter estimates for a conceptual catchment model applied to a series of small- to medium-size catchments. The question of when such measurements should be taken to provide a maximum of information, and how to predict these times in advance, remains. *Montanari and Toth* [2007] showed how short and fragmented hydrological time series can be effectively used to calibrate hydrological models with spectral techniques. Another alternative is the use of soft information to provide a first assessment of what watershed behavior might be expected. For instance, *Seibert and McDonnell* [2002] use soft information to set up, calibrate, and further test a conceptual catchment model. The latter was a first step toward quantifying process understanding so that it can be used in watershed modeling, a strategy still largely untapped for PUB thus far.

[16] Finally, in the absence of any local information on hydrologic variables and if no regional regression can be performed because of a scarcity of gauges, then it might still be possible to achieve some bracketing on selected signatures through theoretical argumentation. Examples could be analytical solutions to the Budyko curve [e.g., *Gerrits et al.*, 2009] or base flow recession characteristics from idealized aquifers [e.g., *Brutsaert*, 2005]. Such theory might at least provide some guidance on how watershed models, with significant flexibility in simulating real-world systems, should not behave.

[17] Once distribution functions of one or more signatures have been established, different approaches can be used to assimilate this information into a watershed model. Basically, if we have selected a watershed model and parameter priors, then we can sample from this feasible parameter space and create an ensemble of predictions of streamflow. From each streamflow prediction, we can also derive a prediction of the signatures that have been independently calculated for the watershed at hand. Ensemble members that produce signatures closer to the expected signature values are more likely to be representations of the watershed behavior than those that are farther apart. Closeness of simulated signatures to model-independent signatures PDFs can be assessed following two main pathways, either using a set theoretic strategy [e.g., *Yadav et al.*, 2007; *Zhang et al.*, 2008; *Liu et al.*, 2009; *Winsemius et al.*, 2009] or using a more formal approach [e.g., *Bulygina et al.*, 2009, 2011; *Castiglioni et al.*, 2010]. The differences between the two basic strategies to estimate predictive uncertainty (and their scientific validity) have been discussed elsewhere [see *Montanari*, 2005; *Mantovan and Todini*, 2006; *Beven et al.*, 2008; *Stedinger et al.*, 2008], and we do not want to repeat this discussion here.

[18] While some might view the sampling of the feasible parameter space for behavioral parameter sets as a minor technical issue, it rather represents a potentially large obstacle in using this additional information. In most studies, some form of Monte Carlo random sampling has been used to find behavioral parameter sets [e.g., *Yadav et al.*, 2007; *Winsemius et al.*, 2009; *Bulygina et al.*, 2009, 2011]. However, the search space could be rather complex because of the possible simultaneous use of several signatures, the potential error in the estimates of the signatures, the correlation between the signatures, and (unknown) model structural and data error that might limit the model's ability to reproduce the signatures. In addition, the watershed model could be quite complex and hence exhibit a high-dimensional parameter space. *Zhang et al.* [2008] reviewed this problem in detail and showed how the search for behavioral simulations (and hence for behavioral parameter sets) can be reformulated as a multiobjective optimization problem. Using a genetic algorithm, their study showed a tremendous gain in efficiency

in identifying a population of behavioral parameter sets as defined by constraints on three hydrologic signatures. Other studies optimized watershed models to regionalized streamflow characteristics at ungauged locations as well, though without explicitly accounting for uncertainty in the regionalized indices [e.g., *Bárdossy*, 2007; *Castiglioni et al.*, 2010].

5. Opportunities and Open Research Questions

[19] In our opinion, this change in focus away from concentrating on the watershed model alone toward better utilization of our understanding of watershed behavior represents an important advancement in the predictions in PUB strategy. Previously, the estimation of hydrologic signatures at ungauged locations had generally been seen as separate from watershed modeling, typically confined to the area of statistical hydrology and engineering, and process knowledge has been underused. Both sources of information now represent one part of a two-pronged strategy combining both a priori information on the model and a priori information on the watershed dynamics into a single strategy. This shift opens up new opportunities for collaboration between hydrologists focusing on statistical, experimental, and modeling approaches to understand the hydrologic similarity between systems, an understanding that forms the basis for any kind of information transfer [*Wagener et al.*, 2007].

[20] What behavior do we expect an ungauged watershed to exhibit? While the research provides a first step toward using this additional source, many questions remain and provide exciting research challenges. They include the following.

[21] 1. How many signatures (and which ones) are required to define the dynamic hydrological behavior of a watershed?

[22] 2. What are the signatures of watershed function (dynamics) that can be derived in the absence of local streamflow observations in view of recent progress in observation techniques (e.g., remote sensing or gravity measurements)?

[23] 3. What observations of internal flow paths and residence times (e.g., using tracers) are available at enough locations to understand controls on hydrologic signatures with more descriptive power than those derived from streamflow?

[24] 4. How can probability distribution functions for different signatures best be estimated (e.g., regionalization versus short-term measurement)?

[25] 5. Given that any additional information brings additional uncertainty, what is the best strategy to identify "informative" signatures, namely, information that effectively allows one to reduce simulation uncertainty?

[26] 6. Assuming that more complex models contain more information about the watershed, how does the number of signatures required for uncertainty reduction change with changing model complexity? Can we show that more complex models contain more "knowledge," and if so, how much more?

[27] 7. Can we quantify the learning that occurs through new understanding as evidenced by a tightening of the probability density functions that describe dynamic watershed behavior?

[28] 8. How do we efficiently find behavioral models (parameter sets) in these potentially high-dimensional and complex parameter (maybe even model structural) and signature spaces?

[29] 9. How do we separate model structural error (i.e., the ability of the model to reach the signature space) and data error from potentially wrong PDFs of the watershed signatures?

[30] 10. What is the best strategy for merging signatures and models? How much do the final results between Bayesian and set theoretic approaches actually differ?

[31] 11. Can we provide the user with an indication of the simulation reliability? That is, where and when can we expect simulations and/or uncertainty estimates to be more or less reliable in a particular ungauged watershed?

[32] 12. Can we use cases of conflicting information (signature versus model) to improve methods or models?

[33] Understanding variability and controls on signatures requires the analysis of many watersheds. However, there is a trade-off between the depth of the analysis and the number of watersheds that can be included in a study. Both variability and depth are ultimately required. Studies to understand controls on hydrologic signatures across a smaller region, where the trade-off between heterogeneity and depth is smaller, will be especially helpful in this regard [e.g., *Tague and Grant*, 2004; *Beighley et al.*, 2005; *Tetzlaff et al.*, 2009], and more are needed. Another need lies in the meta-analysis of studies from multiple regions, something not often done in hydrology, which have the potential to better understand transferability (and maybe generality) of conclusions. Finally, signatures may also allow us to gain understanding about the temporal evolution of watershed behavior under changing climate or land use characteristics through a better understanding of controls on spatial gradients of hydrologic signatures; that is, a trading space for time strategy could be used [*Wagener*, 2007; *Buytaert and Beven*, 2009; *Bulygina et al.*, 2009; *Blöschl and Montanari*, 2010].

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