HESS Opinions

"Advocating Process Modeling and De-Emphasizing Parameter Estimation"

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Abstract

Since its origins as an engineering discipline, with its widespread use of '*black box*' (empirical) modelling approaches, hydrology has evolved into a scientific discipline that seeks a more '*white box*' (physics-based) modelling approach to solving problems such as the description and simulation of the rainfall-runoff responses of a watershed. There has been much recent debate regarding the future of the hydrological sciences, and several publications have voiced opinions on this subject. This opinion paper seeks to comment and expand upon some recent publications that have advocated an increased focus on process-based modelling while de-emphasizing the focus on detailed attention to parameter estimation. In particular, it offers a perspective that emphasizes a more hydraulic (more physics-based and less empirical) approach to development and implementation of hydrological models.

1 Introduction

There has been a recent call in several notable publications for a new focus to be brought to the hydrological sciences. As an example, *Montanari et al. (2015)* stressed the need for new vision, to help drive new theories, new methods and "new thinking". This comes at a time when enhanced computational power and sophisticated monitoring techniques now enable hydrologists to pursue deeper investigations of hydrologic processes, and to thereby simulate watershed hydrology in ever more detail.

It is my opinion that we need to take a broader look at the practices we bring to hydrological modelling. My experience suggests that we too often allow ourselves to become mired in relatively minor problems, and thereby fail to notice some of the more major ones. For example, do we not tend to become over-focused on estimating parameter values by "optimization", and should we not instead devote more of our focus to improve the models that represent the underlying system processes? Is it not possible to conduct model evaluation (as a support for model building) in a much more intellectually satisfying manner? This paper, while commenting on and referring to some related publications, seeks to promote discussion of such questions and advocates the need for enhanced focus on understanding and representing hydrological processes accurately, so as to improve our conceptual understanding and even our hydrological perceptions.

2 On model parameterization and the need for parameter optimization

In a recent debate on the future of hydrological sciences, and in the context of a discussion of modeled process parameterization and parameter estimation, *Gupta and Nearing (2014)* state that "*we suggest that much can be gained by focusing more directly on the a priori role of Process Modeling (particularly System Architecture) while de-emphasizing detailed System Parameterizations*". Soon after, *Gharari et al. (2014)* presented a practical and methodical demonstration that the need for model calibration (optimization of parameter values) can be dramatically reduced (and even avoided) by the judicious imposition of (both general and site-specific) relational parameter and process constraints onto our models. They report that doing so can significantly improve the results while reducing simulation uncertainty.

The arguments and demonstration mentioned above are recent contributions to a long-standing perspective held by others in the hydrological community. *Bergstrom (2006)*, for example, based on his experience with the HBV model as a solution for prediction in ungauged basins, mentions three possible ways that runoff in rivers can be estimated in the absence of directly available data. "*The first was to simply use information from neighboring rivers through statistical methods. The second option was to get so much experience with a conceptual model that we can map the optimum values of its parameters, or relate them to catchment characteristics. The third* *was to use a model that is so physically correct that it does not need calibration at all*" (*Bergstrom, 2006*).

My own experience, based on working with a physics- and GIS-based fully distributed hydrologic model called WetSpa, is similar to the second aforementioned option proposed by *Bergstrom (2006)*, and resonates with the "*limited need for calibration*" shown so nicely by *Gharari et al. (2014)* (see also *Hrachowitz et al. 2014*). I have found that the need for parameter calibration can be dramatically reduced simply by avoiding the now-common "*trial and error*" strategy of search by optimization, and proceeding instead by a) beginning with some reasonable initial values derived based on known catchment characteristics, b) some trial and error to refine the reasonable initial values, and c) proceeding to imposing some meaningful and sensible constraints and parameter relational rules. I find that, much of the time, excellent parameter values (and hence model performance) can be obtained in only a few attempts and without considerable effort. With some degree of practice, and after gaining some understanding about how the hydrological processes are represented in the model and how the parameters relate to observable or conceptual catchment characteristics, the process of model calibration is eased to such an extent that it would imply that the model needs no parameter calibration but only a kind of parameter "*allocation*" (i.e., a logic-based specification); I will discuss parameter allocation in detail later in this paper.

According to *Beven (2000, 2006, 2011)* and *McDonnell and Beven (2014)* the importance of uniqueness of place and the limitations of hydrological data can, in most cases, make parameter allocation rather difficult, and so we should consider the limitations of current concepts. As mentioned by *Beven* in his referee comment, in practice we are both model and data limited, and even a perfect model will be limited by inconsistencies in the calibration and prediction data (e.g. *Beven and Smith, 2014*) – so that the success or failure of a model run with a priori parameter estimates might depend more on the (unknown) errors in the data than on whether the model is a realistic representation of the processes.

However, the work of Bergstrom with the HBV model, and more recently *Semenova and Beven (2015)* seems to suggest otherwise (although note that Beven has a different opinion in this regards, as discussed briefly in their paper; see also Beven's equifinality thesis in *Beven, 2006b*). The work of the St. Petersburg modeling team on a deterministic distributed process-based model of runoff formation processes named "hydrograph model" is closely in line with what is described for parameter estimation in this opinion paper (*Vinogradov, 1990, Vinogradov et al. 2011, Semenova et al. 2013 and 2015, Lebedeva et al. 2014*). In their approach, they "do not accept calibration in the form of automated procedure of parameter estimation", and "assume its common application to be one of the main barriers in development of modern hydrological modeling" (www.hydrograph-model.ru).

It seems, in fact, that it may often be possible to arrive at parameter values through a process of reasoning and white box modeling, rather than by the inefficient and poorly informed search procedures involved in trial-and-error or black box efforts. As another example of the use of knowledge from processes to constrain parameters in a physically based, spatially distributed model, I note the TOPKAPI modeling work of *Ragettli and Pellicciotti (2012*) in a glacier-dominated basin; their report includes an evaluation of the transferability of such parameters in time and space.

To estimate the parameters of a spatially distributed flash flood model, *Blosch et al. (2008)* have emphasized understanding the model behavior over formal calibration. Similarly, *Merz and Blosch (2008a, 2008b)* and *Viglione et al (2013)* provide good examples of the use of hydrological reasoning to obtain more informed estimates of flood frequencies, and *Hingray et al. (2010)* present a signature-based model calibration for hydrological prediction in mesoscale Alpine catchments. In the latter, the calibration method uses hydrological process knowledge to extract useful information from very heterogeneous data set available in the region (see also *Schaefli et al., (2005)* and *Schaefli and Huss (2011).*

In other work, *Vidal et al. (2007)* reviewed the process of calibrating physically-based models such as river hydraulic models and distributed hydrological models with a special emphasis on knowledge base calibration. They criticize the fact that calibration is often done without any or with only minimal physical consideration. They advocate a definition of parameter calibration "on the basis of heuristic knowledge gained through modeling experience", and develop a knowledge based calibration support system for hydraulic modelers. The result is an automatic knowledge-based trial and error approach that also has the advantages of reliability and reproducibility. The resulting CaRMA-1 algorithm mimics the way that experts tackle particular calibration cases to obtain the most reasonable calibrated hydraulic model considering the data available. Other examples of limited calibration (parameter adjustment) and hydrologic reasoning for parameters estimation of physically based distributed models can be found in *Feyen et al. (2000)* using MIKE SHE, *Zehe and Bloschl (2004)* for parameter adjustments of CATFLOW, and *Bahremand et al. (2005, 2007), Liu et al. (2003, 2005)* with the WetSpa model, and *Salvadore (2015)* with the WetSpa-Python model.

Some recent publications regarding conceptual hydrologic models have also drawn attention to the use of expert knowledge in parameter estimation and constraining parameter calibration; see for example *Antonetti et al. (2015), Hrachowitz et al. (2014), Gharari et al. (2014), Hellebrand et al. (2011)* and *Viviroli et al. (2009)*. Overall, the examples mentioned above lend support to the author's conviction that by gaining some understanding about hydrologic processes, and by trying to relate the parameters to observable (or conceptual) watershed characteristics, it is possible to infer reasonable values for the parameters of a hydrological model.

In support of this viewpoint, let us look at some examples using the WetSpa model, which has 11 parameters that must be specified (*Liu and De Smedt, 2004*). As a trivial case, consider the parameter Kg_m that represents the maximum active groundwater storage (in mm) and controls the amount of evaporation possible from the water table. This parameter has typically been considered to be "*insensitive*" (see *Bahremand and De Smedt, 2008*), which makes sense of course if the catchment is mountainous and in an upstream area (e.g., catchment order 2), because logic dictates that since the depth to groundwater is so deep, there will be little or no direct evaporation from the water table. In such a case we can save time by fixing this parameter to a large value, and directing our attention to other aspects of the model. Similar reasoning can be applied to several other parameters (*Bahremand et al. 2007, Liu et al. 2003*).

Alternatively, if the practitioner prefers to proceed with an automatic calibration approach (although I prefer the manual calibration approach due to its ability to enhance hydrologic knowledge), much is to be gained by advising her/him to implement some logical relativity restrictions. For example, in the WetSpa model it makes sense to always restrict the value for parameter Kg_i (initial active groundwater storage, in mm) to be less than the value for Kg_m. Doing so helps to restrict the calibration search space, so that the "*best*" parameter values are achieved with the least effort, and the parameter values remain relatively consistent with their conceptual meaning. A nice example of this is provided by *De Smedt et al. (2000)* who implement such reasoning in regards to the parameter values (based on an understanding of the physical structure of the model) and obtain quite good model simulation results without resorting to any "*calibration*". In support of this, note that *Safari et al (2012)* reported satisfactory results using an uncalibrated WetSpa, with only minor improvements obtained through calibration (see also *Smith et al. 2012*). *Zeinivand and De Smedt (2009, 2010)* reported results of the snow modules of the WetSpa model using preset values with no calibration.

Other "no-calibration" modeling studies using physically-based distributed hydrologic models have reported mixed success (e.g., *Semenova et al. 2015, Venogradov et al. 2011, Refsgaard and Knudsen 1996,* and *Refsgaard et al. 1999)*. Here, "no-calibration" refers to the use of preset parameter values, and "limited-calibration" is taken to mean "manual adjustment … applied to a small group of specially chosen parameters … … carried out as a priori defined narrow ranges of parameter variation…" (*Vinogradov et al. 2011*).

Examples of limited calibration of the WetSpa model are given by *Liu (2003, 2005)* and *Bahremand (2007, 2005)*. I think of such an approach as being a kind of "*white box calibration*", and my experiences with the WetSpa model (*Bahremand et. al 2005 and 2007, Bahremand and De Smedt, 2008 and 2010*) suggest that it can help to ensure a considerable degree of consistency in both the parameter values and the model behavior. As discussed later in this paper, other no-calibration attempts for physical modeling have been reported using the novel approach of optimality (*Schymanski et. al. 2009*), maximum entropy production (*Westhoff and Zehe, 2013*), and behavioral modeling under organizing principles (*Schaefli et al. 2011*).

Of course, when a user selects reasonable initial values for the automated local parameter search, this is akin to bringing some kind of informed prior information to bear on the calibration process, in a manner similar to Bayesian inference, or the expert opinion in decision-making. Accordingly, it helps to improve calibration efficiency, results in enhanced parameter consistency, and reduces uncertainty, thereby improving the overall result. Similarly, in a regionalization process, we bring to bear our prior knowledge about the nature of the catchment and the dominant processes within it to minimize (and if possible, avoid) the need for model calibration and parameter estimation tasks. Via a process of generalization, we find ways to apply our models in ungauged basins based on parameter maps that relate catchment characteristics to parameter values via a combination of expert knowledge and empirical evidence (*Bergstrom, 2006; Bardossy, 2007*). And, in the case of expert opinion used to guide decision-making we employ a similar practice

The point is, that in all of the cases, there is a greater emphasis on process understanding, and as such understanding is enhanced, the parameter estimation problem becomes progressively more trivial. As stated by Hoshin Gupta in a recent email communication (email communication, 31 March 2015), "*it is good to give the students a well-organized frame to think about the model development process because, it can dramatically help to reduce the effort. In my opinion we (the community) have taken a journey of about 30 years long to "rediscover" this because in the late 70's and 80's we were seduced by the ideas of "optimization" (which came from operations research) and the ability to play with computers. Hopefully now the field of "systems hydrology" will focus more on what I like to call the "learning problem" - which is more about architecture and process parameterization than about parameters. Of course some amount of calibration will generally help because the model is always a simplification*".

3 On the Model development process

The model development process follows a series of several steps. Since these steps have been discussed variously by *Beven (2012)*, *Gupta et al. (2012)*, and *Gupta and Nearing (2014),* among others, the reader may refer to those articles for details. I mention them only briefly here. As mentioned by *Gupta et al. (2012)* first stage is informal and involves the formation of "*perceptions*" about the system. In the formal steps, we begin with a "*conceptual model*", and then proceed (in the language of Beven) to develop a "*procedural model*" (but see *Gupta et al., 2012* for considerably more fine-grained detail). Finally we run the model with some initial parameter guesses, and then proceed with model calibration and evaluation, sensitivity analysis and uncertainty analysis. These last 4 steps can perhaps be grouped under the general term of "*model optimization*".

The important step that follows is that of model "*verification*" (or perhaps we can call this diagnostic evaluation and improvement; see *Gupta et al., 2008*). In *Beven (2012)* is implied by the word "*revise*" (in the second illustration of the first chapter of Beven's book). We advise the practitioner that if the constructed model "*fails*" the diagnostic evaluation step we should first revisit the calibration step (just one step back) to check whether we could do better by calibrating our model differently. If everything is found to be “ok” in this step, we should proceed backward one more step and take a closer look at the “*procedural model*”, to check the computer code for errors. And, if this seems fine we can proceed to examine our “*conceptual model*”, whereby we check the equations used, the manner in which subsystems are linked to each other, inputs, outputs, functions, and so on. Finally if everything seems fine, then we may be forced to question our perceptions, examining in detail how we have defined the processes.

However, the current modeling practice seems to be largely stuck in the model optimization stages. *Gupta and Nearing (2014)* correctly suggest that we have given more than enough attention to the problem of model optimization. And several authors have argued that if we want to have real improvements in modeling practice and performance, then we need to take a more serious look at the early steps in the modeling protocol, and in particular focus in on the "*process model*" (even being willing to alter our perceptual model).

It is instructive to note that, despite the diversity in hydrological behaviors found in catchments of different kinds, most current conceptual watershed models are only slightly different implementations of very similar perceptions and conceptions in regard to watershed behavior, and involve very similar kinds of simplifications and assumptions. In this context, novel ideas such as HAND and the topographic index embody interesting revisions in the perceptual and conceptual model stages of conceptual-hydrologic modeling (*Savenije, 2010; Gharari et al., 2011; Gao et al., 2014*). Similarly the REW approach is an example of revisions in early stages of physical-hydrologic modeling (*Reggiani et al. 1998 and 1999)*. And as suggested by *McDonnell et al. (2007)*, "*New approaches should rely not on calibration, but rather on systematic learning from observed data, and on increased understanding and search for new hydrologic theories*". It is, of course always easier to improve upon an already existing model/framework. In some cases, however, really significant improvements can only come about by starting at the very beginning. In my view, the end of optimization can serve as a new beginning for the hydrological modeling process.

4 On the modeling and evaluation of hydrologic processes

It seems obvious that hydrologists should be ready to investigate our perceptions and be willing to make dramatic improvements in conceptualizations as needed. Various assumptions, expediencies and simplifications may need to be changed or disregarded. As mentioned by Grey Nearing in a recent email communication (email communication, 31 March 2015), "*It is strange that we know a priori that any model we build will be incorrect, and so the pertinent question in my mind is in what sense a wrong model can be useful. Since calibration can never fix the fact that our models are always wrong, we must interpret the calibration procedure as in some sense reducing the impact of our model's errors on the utility of that model. Neither calibration nor iterative model refinement will ever result in a correct model, and error functions, likelihoods, objective functions, and performance metrics are all attempts to measure model utility, not model correctness. My opinion is that this utility approach to model building and model evaluation is misguided. Instead of building a model that we know is wrong and then trying to estimate how wrong it is, we should try to use our knowledge of physics to constrain the possibilities of future events. That is, instead of trying to approximately solve complex systems of equations, use the equations to limit the possibilities of future events. Shervan Gharari takes this perspective to assigning parameters in his recent paper (Gharari et al., 2014), and for this reason it is one of my favorite*".

While Nearing argues that the *current* paradigm is based fundamentally around a concept of utility, and that our knowledge of physics should be used to constrain the possibilities of future events, Gupta refers to such a focus as "*prediction and problem solving, and to serve such purpose while improving our understanding of "physics", so the target becomes the "model" and this sets up a recursive loop when we try to "support/evaluate" the model*."

In practice, I have found a ladder type (tree-like) evaluation and model intercomparison framework (of flexible length) to be useful for model evaluation. In the short version of this ladder, the modeler is able to "*evaluate/support*" a particular model by seeking, for example, an improved simulation of the total hydrograph. Given a lumped conceptual model “A” and a physics based distributed model “B”, the short ladder evaluation allows us to compare the hydrographs simulated by A and B with each other, and with the observed target data. This kind of evaluation really just serves the model, in the sense that it supports the specific kind of prediction needed by a target application such as river hydrograph simulation/prediction.

In contrast, the long version of the ladder can take us much deeper. In this type of evaluation, our goal is not model intercomparison based on target performance, but is instead based on consistency or realism. For example, in the first step (stair/stage) we have a descriptive table that enables comparison between the conceptualizations underlying the models. It enables us to compare which hydrological processes are represented in the models, and how they are interlinked (although this latter could perhaps be considered a second step). In such a context, it does not really make sense to compare an artificial neural network black box type model against a fully distributed physically-based model, which comparison could mislead a naïve practitioner (being a comparison between two different kinds of things).

Ultimately, we need to develop frameworks for model evaluation and comparison that enable us to give more weight to ones that better represent the underlying physics (see *Clark et al., 2011; 2015a,b; Mendoza et al., 2015*). This kind of long ladder evaluation enables us to progressively deepen our understanding, step by step. Along the way, some models may be left behind, but can continue to serve our immediate and intermediate needs such as for hydrograph simulation. However, later steps may require our model to pass additional tests, such as requiring the flow velocity in streams of order 1 and located in forested terrain to be meaningful in comparison with the velocities in similar streams passing through high altitude farmland.

In such a context, a simple hydrograph comparison may generally not be sufficient, and simple model efficiency and performance metrics on streamflow will not guarantee that the system has been correctly described (*Klemes, 1986; Bergestrom, 1991;* see also *Savenije, 2009* for a discussion of what constitutes a "*good model*"). So, for example, the behavioral and non-behavioral models partitioning within a GLUE framework (*Beven and Binley, 1992*) should not be based simply on model output-based performance criteria, but should be meaningful and correct in an intellectual manner. The use of relational rules (as in *Gharari et al., 2014*) serves the function of prior information.

As has been pointed out in the literature, our approach to model evaluation that is based in performance criteria also needs improvement. Recent work in this regard includes the Kling-Gupta efficiency (*Gupta et al., 2009*), the increasing emphasis on process/signature-based diagnostics (*Gupta et al., 2008; Yilmaz et al., 2008*), and the use of multi objective criteria and evaluation on multiple variables (*Gupta et al., 1998; Pechlivanidis and Arheimer, 2015*). Equally important, we need to establish benchmark problems that serve as a set of standard test cases, thereby providing the modeling community with a way to perform fair assessments of competing formulations, parameterizations and algorithms (*Maxwell et al., 2014; Paniconi and Putti, 2015*).

Ultimately, model optimization can help establish the best possible model performance compared with input-output data, uncertainty analyses can help to reveal model structural deficiencies, and comparison against benchmark prediction limits (e.g., *Schaefli and Gupta 2007*) can provide a possible way of checking the correctness of our understanding of the hydrological processes at a given time and place (*Montanari and Koutsoyiannis, 2012*). While this may be obvious to an experienced modeler, I feel that we should be thinking about building a structured framework that can help beginners/students to stay on the right track, and not be deceived by "good" values of summary metrics such as the Nash-Sutcliffe Efficiency. In such a structured framework, it will be important to take first into account model simplifications, assumptions, formulations, the code, and the list of processes, before examining the simulation results. And, an automated model calibration procedure should not be used as a way to justify a poorly formulated model that is then "*camouflaged by uncertainty estimation*". As has been pointed out before many times (see e.g., *Semenova and Beven, 2015*), expert opinion and judgment should matter when evaluating the credibility of model performance and predictions. To this one might add that scientific knowledge and principles of physics should matter even more, as should practical perceptual and observational knowledge about the system being modeled.

As examples of the latter, consider the following. Although flow widths change along the stream network, most hydrological models use a constant width for the stream network; at the very least, streams of different order should be allocated different widths. Most hydrological models assume constant flow velocity fields for the entire duration of the simulation; in fact, flow velocities should be considered together with the sediment and bed loads. Similarly, hydrological flow routing should take into account transmission losses, the differences between velocities and celerities, hysteresis with respect to total storage in a landscape element, heterogeneities and the extremes of their distribution. To quote *Semenova and Beven (2015)*, "*These are requirements for any distributed modeling scheme in hydrology that is going to be intellectually satisfying in reproducing both flow and travel times of water*". Doing so will bring to bear well-known hydraulic principles. Bringing physics and more detailed attention to process modeling will also leads to better integration of surface and subsurface hydrology in models (*Paniconi and Putti 2015*).

Moreover, alternative theories and approaches, such as representative elementary watershed concept of *Reggiani et al. (1998 and 1999)* and the thermodynamic reinterpretation of the HRU concept of *Zehe et al. (2014)*, help us to limit uncertainty and better deal with equifinality by improving our understanding of the system. Although even physics based models face equifinality (see *Klaus and Zehe, 2010; Weienhoefer and Zehe, 2014*), as this problem simply arises from the structure of our equations (see *Zehe et al., 2014*), by explicitly disentangling driving gradients and resistance terms in flow equations the process-based models offer more options to exert constraining rules to end up with a rather unique parameter set (*Zehe et al., 2014*). Taking more processes into account decreases non-uniqueness, as for example *Wienhöfer and Zehe (2014)* reduced "the number of equifinal model set-ups" by the results of solute transport simulations.

Also, some processes such as subsurface processes and preferential flow need to be better represented explicitly, and we should consider the limitation of Darcy-Richards equations (being diffusive and assuming local equilibrium conditions) regarding the fast advective responses and cell size limitation (*Vogel and Ippisch, 2008*). Similar to the multi-objective criteria approach in model optimization, where a set of criteria is involved in the search for a unique parameter set; accordingly from a different angle, if we take more physical processes into account into our model structure, it does a similar thing, i.e. it gives us more options to constrain parameter values and reach a rather unique parameter set. Therefore, the equifinality should be dealt with from different angles to help us to arrive at a better model.

Another approach to dealing with equifinality is by limiting the parameter values through a procedure that can be called parameter allocation. In the following section, I express my ideas in this regard and on the future of hydrological modeling.

5 On parameter allocation and the future of hydrological modelling

In this section, I articulate my opinions regarding parameter allocation and the future of hydrological modeling, and in particular my opinion in regards to physically-based distributed models as the right path to model hydrologic processes and to avoid calibration and its related uncertainties.

5.1 Contrasting parameter calibration and parameter allocation

In the process of model development, calibration seems unavoidable (*Beven, 2001; Montanari and Toth, 2007; Hrachowitz et al. 2013*) as a way to compensate for our lack of knowledge of spatial heterogeneities in watershed properties and our lack of understanding of hydrologic processes (*McDonnell et al. 2007*). It can be done either manually or automatically or by some hybrid approach (*Boyle et al 2000, Hogue et al 2000, 2006*). Manual calibration applies hydrologic knowledge and reasoning to obtain the good parameter values in fewer attempts but involves trial and error and is very time consuming. Automated calibration approaches may not add much to the hydrologic knowledge of the practitioner, but can be very helpful when there are many parameters to be determined (overcoming the tedium and time involved in manual calibration), provides the possibility of quickly checking numerous combinations of plausible parameter values (that would be impossible to attempt manually), and can provide useful support to model diagnostic evaluation. Indeed, when the best parameter estimate is physically unrealistic, one may conclude that the model is not adequate, and such a conclusion can only be reached if an exhaustive search for the best parameter estimates has been carried out (see Montanari's referee comment on this paper; *Gupta et al. 1999*). Since, automatic calibration is an iterative procedure, it also provides information useful for parameter sensitivity and uncertainty analysis *(Bahremand and De Smedt, 2008)*. As explored by *Boyle et al (2000)* and *Hogue et al (2000, 2006)*, a hybrid combination of these two types of calibration approaches is also possible.

Meanwhile, what I refer to here as parameter "allocation" does indeed play an important role in hydrological modeling but has not received sufficient discussion although it is something that experienced modelers typically do in any modeling study (see Schaefli's referee comment on this paper). I argue that this aspect deserves more attention, since it is in the direction of achieving more understanding of the hydrological processes, the way they are represented in the model, and the link between model parameters and catchment characteristics (this understanding can be extended to conform with the organizing principles mentioned in *Schaefli et al., 2011*).

Parameter allocation is relevant in the case of process-based models, whose parameters are more likely to have physical or conceptual meaning and be rationally explainable. With some degree of practice, and after having gained some understanding of how hydrological processes are represented in the model and how the parameters relate to observable or conceptual catchment characteristics, the modeler can specify values for the parameters based on logical reasoning. Of course, for some of the parameters, a few trial and error adjustments might still prove to be necessary and useful. It is, therefore, a heuristic technique, a kind of ansatz, in which an educated guess is made regarding the parameter values, which can later be verified through an evaluation of the model performance.

So, parameter allocation can be viewed as a part of (or kind of) the parameter calibration procedure. Whether using a manual or automatic approach, the modeler can use rationality and logic (based mainly on hydrologic reasoning) to guide parameter improvements. Reasoning can be used to establish constraints and relational rules between parameters, in accord with relevant organizing principles (this needs to be elaborated via future modeling research), and in accordance with a higher level (global or regional) water balance model. These latter two (conformity with organizing principles and water balance scheme) are particularly relevant when attempting to develop a community hydrological model (*Weiler and Beven, 2015*) or a hyper resolution model of everywhere (*Beven, 2007, 2015, Beven and Alcock, 2012*). Such constraints and relational rules can either be applied manually, or by some computer-based procedure (see *Gharari et al. 2014; Vidal et al. 2007*).

Essentially, what makes the difference between parameter "allocation" and parameter "calibration" is the extent of prior knowledge applied by the modeler. In parameter calibration, prior knowledge is mainly used to set the allowable range of parameter values (to establish the "feasible" parameter space). In parameter allocation, additional prior knowledge is imposed in the form of relational rules between parameters, some certain constraints and principles. In this case, the modeler does attempts to allocate values for as many of the parameters as possible, so that the need for trial and error adjustments is minimized and limited to only a few parameters.

The point is, of course, to make as much use of prior knowledge as possible, so as to limit/minimize the uncertainty, while arriving at reasonable (physically or conceptually defensible) values for the parameter, ones that support our basic conceptual understanding of the system. In this context, models with the smallest number of "parameters-subjected-to-calibration" will be considered more scientifically interesting, and parameter estimation becomes part of the learning process (see comment by Hoshin Gupta mentioned above). The primary motivation and emphasis becomes "understanding" rather than "good results"; i.e., less accurate results with reasonable parameter values (and model behaviors) are more desirable than more accurate results with unreasonable parameter values. It brings to the foreground the need to make a tradeoff between accuracy and reasonability, given the fact that every model is a simplification of reality.

Below, I outline a few steps that can be followed in the parameter allocation procedure for a physics based model:

I) Conduct a preliminary rough evaluation of parameter behavior or sensitivity (an optimum parameter set from a previous study in a different catchment can be a good choice to start with). The modeler is supposed to understand how the model response relates to the values of its parameters, and such a test helps to verify the expected behavior for the new study area.

II) Specify (allocate) values for those parameters for which approximate values can be easily established by following rules of thumb (like parameters Kg_i and Kp in the WetSpa model, see *Bahremand and De Smedt, 2008* for the model parameters).

III) Fix any "insensitive" parameters to reasonable nominal values. This step may not generally be necessary for physically-based distributed models, because their parameters are usually likely to be sensitive; however, in my work with the WetSpa model, I found it appropriate to fix one insensitive parameter (parameter Kg_m). Similarly *Roux et al. (2011)* and *He et al. (2015)* also report fixing insensitive parameters of their physically based models (MARINE and THREW).

IV) Allocate approximate values for parameters that show consistent relational behavior with catchment characteristics (e.g., parameter Kg in the WetSpa model, see *Bahremand et al. 2005, 2007*, *Liu et al. 2003, 2005*).

V) Collect and list all of the relational inequality constraints between parameters (e.g, $Kg_i < Kg_m$ in the WetSpa model), the conceptual relations between parameters and catchment characteristics, (as well as organizing principles and water balance related constraints).

VI) Apply inequality conditions that may be relevant between some of the parameters. Those parameters having constraints and relational rules are allocated together. The constraints can be either implemented manually or using simple computer codes in case of automatic procedure (see, for example, the tool presented by *Vidal, 2007*).

VII) In some cases, the model parameters and/or processes will be required to conform with organizing principles such as optimality, landscape evolution laws, and Horton laws of stream networks (e.g. Horton number of bifurcation); and a higher level water balance model (a regional or global model) should be satisfied. As an example of the latter, *Schaefli and Huss (2011)* used glacier mass balance data to constrain the parameter uncertainty for their hydrological model in a glaciered basin (see also *He et al. 2015*). For the purpose of developing a community hydrological model, a universal water balance model can be used to establish constraints on our local model and its parameters. Another way to say this is that while our models are calibrated locally to observations, they must also obey parameter inter-relationships and constraints, and the organizing principles and components of a universal water balance model. These three different types of constraints (i.e, constraints between parameters, organizing principles, and balance related controls) will allow us to pre-set most of the parameters. However, the idea behind this step still feels somewhat "rough" in my minds, and needs further elaboration and perhaps revision.

As mentioned above, for some of the parameters the results will be a parameter range rather than a definite value, and it is likely that some residual manual trial and error adjustments may still be necessary before the modeler can decide on the final parameter values. Having arrived at this "allocated" set, one must trust in, and be confident with, the outcome.

5.2 Some further comments regarding parameter allocation

My experience with this kind of parameter allocation is that it has attributes of both the bottom-up and top-down approaches to model development. By this, I mean that the modeler is required to be able to change her/his viewpoint based on what happens during the parameter allocation process. The manual-expert and automated approaches each have their advantages and disadvantages, and an experienced modeler brings both approaches to bear when seeking to allocate values for the parameters. In this way, the process can act as a link between deductive physics-based distributed modeling and the behavioral modeling approach (using organizing principle to constrain models) described by *Schaefli et al. (2011)*.

Whereas parameter allocation can be used to establish relatively narrow ranges on the parameter values, the application of optimality or organizing principles can help to further restrict these ranges. *Schaefli et al., (2011)* express this as "*adjusting the model structure and parameters so as to respect this organizing principle*". Some that have received attention in the literature include the optimality principle (*Schymanski, 2008 and 2009*), maximum energy dissipation (*Zehe et al. 2010*), maximum entropy production (*Kleidon and Schymanski, 2008; Kleidon et al. 2012 and 2013; Westhoff and Zehe, 2013*), landscape evolution laws and optimal channel networks (*Rodriguez-Iturbe and Rinaldo, 2001; Rinaldo et al. 2013*) or self-organized dissipation of singular events (*Beven 2015).* Proper application of such principles can be used to improve the theoretical underpinnings of hydrologic models *(Clark et al 2016)* and can provide constraints that might be useful in making predictions *(Schaefli et al. 2011)*; although see *Beven (2015)* who calls them purely theoretical conjectures that are difficult to prove. *Schymanski et al. (2009)* presents a good example of how optimality may be a useful way of approaching the prediction and estimation of some vegetation characteristics and fluxes in ungauged basins without calibration.

5.3 On the future of hydrological modeling

To reiterate, hydrological modeling has become more and more physics- and process-based. This opinion paper reflects my passion for process-based models, and my (perhaps) radical belief that other types of models do not serve us well anymore. When working with process models, we should spend less time on model optimization and instead focus on our perceptual and conceptual insights with a view to better understanding and expressing the physical nature of the system. This implies that:

1) models should typically only contain physically based parameters
2) models having fitting parameters without physical basis are inferior and should be abandoned
3) spatially-lumped parameters are not physically based and should be avoided
4) models with physically based parameters that are unable to reproduce observations are incomplete or erroneous and need to be improved, fixed or abandoned

5) models with non-sensitive parameters are basically inadequate to simulate the system (i.e., over-parameterization is bad)

6) physical models that “fail” need to be improved, and can help us learn something about what is wrong (impetus for research)

7) in the limit we should strive for “white box models” that do not need any calibration, or only minor calibration (parameter adjustment).

To reach such a goal we need to apply better measurements and better physics. As stated by *Paniconi and Putti (2015),* "*no one would disagree that scientific progress requires a constant dialogue between measurement, analysis, and simulation*". The *Gupta et al. (2014)* paper advocating large-sample hydrology also implies the necessity of such dialog to improve hydrologic science, and *Hrachowitz et al. (2013)* mentions “data” as the backbone of any type of progress.

Of course, both involve significant challenges. *Beven and Germann (2013)* provide a thoughtful discussion on the misuse of physics in simulating flow through porous media, and in particular, the limitations of Darcy and Richards equations; they suggest the representation of preferential flows via a Stokes flow for profile scale and multiple interacting pathways model *(Davies et al., 2011)* at the hillslope scale. *Zehe et al. (2013)* propose a thermodynamic approach to represent catchment scale preferential flow. The mass, energy and momentum balance closure problem presents a significant challenge (*Beven, 2006a*, see also the editor’s comment on my paper), although there has been some progress (*Reggiani et al. 2000, Reggiani and Schellekens, 2003, Reggiani and Reintjes, 2005, Tian et al, 2006, Mou et al. 2008*). *Kleidon and Schymanski (2008*) suggest that the optimality principle can help with the scaling of hydrologic fluxes; knowing the hydrologic fluxes at a larger scale can provide a “big” picture, and a top-down approach can be used to infer the boundary fluxes of ungauged basins at smaller scales.

Perhaps we can describe the future of hydrological modeling by means of an analogy with the problem of solving a spherical jigsaw puzzle, where the puzzle involves assembly of numerous oddly shaped interlocking and tessellating pieces, each having only a small part of the overall picture. To solve the puzzle it is helpful to have 4 different kinds of information:

1) A sense of the complete picture; this can be compared with our perceptual and conceptual model of the hydrologic cycle at the global scale.

2) Information regarding the puzzle edges (borders); this is analogous with large-scale water balance and its components

3) Information regarding the picture expressed by each piece itself; this is analogous to regional or catchment scale hydrological models (the representation of local scale hydrological processes)

4) Information regarding the ways in which the pieces interlock.

It is well known that rapid solution of a jigsaw puzzle can be facilitated by sorting and categorizing the pieces according to shape, color, edge and corner shapes, and shapes of interlocking connectors; this may be comparable with concepts such as generalization, regionalization, and the organizing principles and behavioral modeling of *Schaefli et al. (2011)*. Comparing the partially constructed puzzle with the complete picture (usually printed on the front of the box) is similar to what I have described as a mind commute between the top-down and bottom-up viewpoints (Sivapalan, 2005). The learning process emphasized by *Beven (2007)* in his "*models of everywhere*" and the "*learning instead of rejection*" view exposed by *Gupta and Nearing (2014)* is expressive of this practice. As we continue to work on the puzzle, we try to build upon already completed sections, and eventually we get to the stage where we can see the end of the project where the "holes" become the objects of our attention.

6 Conclusions

In conclusion, it is clear that we need to make a determined effort to shift the focus of our modeling studies away from parameter optimization and towards a deeper attention to process modeling and revision of our conceptual models. We should even be ready to revise our perceptual models. *Gupta and Nearing (2014)* argue that we need robust and rigorous methods to support such a shift, and *Gharari et al. (2014)* shows that such an approach can help to liberate us from the need for model calibration, transforming it into a process of parameter allocation. Ideally, the calibration and evaluation procedures would act synergistically to drive model improvement. Hopefully then, we will move past "*equifinality*" to achieve "equimodellity", reaching at last one fulfilling model that is a "*model that is so physically correct that it does not need calibration at all*"(the third aforementioned solution of Bergstrom). Although such a target might seem unreachable, it could at least act as a beacon for hydrologists.

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