Hydrol. Earth Syst. Sci. Discuss., 12, 12377–12393, 2015
www.hydrol-earth-syst-sci-discuss.net/12/12377/2015/
doi:10.5194/hessd-12-12377-2015
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Hydrology and Earth System Sciences
Open Access
Discussions

This discussion paper is/has been under review for the journal Hydrology and Earth System Sciences (HESS). Please refer to the corresponding final paper in HESS if available.

HESS Opinions: Advocating process modeling and de-emphasizing parameter estimation

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Received: 6 November 2015 – Accepted: 16 November 2015 – Published: 27 November 2015

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Published by Copernicus Publications on behalf of the European Geosciences Union.

Abstract

Since the origins of hydrology as an engineering discipline, where "black box" modelling approaches were common, it has evolved into a scientific discipline that seeks a more "white box" modelling approach to solving problems such as 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 on some recent publications that have advocated an increased focus on process 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 and less conceptual) 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) has stressed the need for new vision requiring 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 parameter optimization, and should we not instead devote most of our focus more to improve modelling of 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 pro-

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mote 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 optimization, 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 that, 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. For example, Bergstrom (2006) 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). 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, and (b) 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).

According to Beven (2000, 2006, 2011) and McDonnell and Beven (2014) "the importance of uniqueness of place and the limitations of hydrological data makes parameter allocation rather difficult in most cases, and we should consider the limitations of current concepts". However, the work of Bergstrom with the HBV model, and more recently Semenova and Beven (2015) seems to suggest otherwise. 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.

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 Kgm that represents the maximum active groundwater storage (in mm) and controls the amount of evaporation possible from the water table. This parameter is typically 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

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directing our attention to other aspects of the model. Similar reasoning can be applied to several other parameters.

Alternatively, if the practitioner prefers to proceed with an automatic calibration approach (which I do not recommend because, in my view, automatic calibration takes the hydrologist nowhere and does not contribute in a significant manner to the enhancement of 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 Kgm. 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". I think of such an approach as being a kind of "white box calibration", and my experiences with the WetSpa model (see Bahremand and De Smedt, 2010) suggest that it can help to ensure a considerable degree of consistency in both the parameter values and the model behavior.

Of course, when a user selects reasonable initial values for the automated local parameter search, this is akin to bringing some kind of wise 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 the 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; Bar-

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dossy, 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 with me (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 1970’s and 1980’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”.

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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 to 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 checking 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 (Savenije, 2010; Gharari et al., 2011; Gao et al., 2014). 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 hydro-

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logic 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 as hydrologists should be ready to investigate our perceptions and be ready and willing to make dramatic improvements in our 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 with me (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, 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

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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

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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 the description of a "good model"). So, for example, the behavioral and non-behavioral models partitioning within a GLUE framework should not be simply based on model output-based performance criteria, but should be meaningful and correct in an intellectually manner. The use of relational rules (as in Gharari et al., 2014) serves the function of prior information. In a recent example, Habibi (2014) applied the GLUE framework to the LISFLOOD-FP model with particular attention to two parameters – the Manning roughness coefficients for the flood plain and for the channel. Out of 500 model runs, 150 realizations were deemed to be behavioral based on an objective function (the F factor). However, closer examination revealed that in 4 of these realizations Manning coefficient for the flood plain was significantly less than the Manning coefficient for the channel, and were therefore non-behavioral.

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 can provide a possible way of checking the correctness of our understanding of the hydrolog-

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ical 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 or 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 celerity's, 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).

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Moreover, alternative theories and approaches such as representative elementary watershed concept of Reggiani et al. (1998, 1999) and the thermodynamic reinterpretation of the HRU concept of Zehe et al. (2014), by improving our understanding of the system, help us to limit uncertainty and better deal with equifinality. 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), but the process based models by explicitly disentangling driving gradients and resistance terms in flow equations 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 needs to be better presented explicitly, and we should consider the limitation of Darci–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 order to reach 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 serve us to reach a better model.

5 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)

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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 can act as a beacon for hydrologists.

Acknowledgements. I would like to thank Hoshin Gupta for his constructive comments and editing the manuscript, and for encouraging me to write and submit my opinion. The paper was significantly improved after being refined by H. Gupta. I owe him a lot. I would also like to thank Alberto Montanari, Grey Nearing, Keith Beven, Shervan Gharari, Claudio Paniconi, Ali Safari, Florimond De Smedt, Yongbo Liu, and Erwin Zehe for their constructive comments on the manuscript and for giving me good direction to better present the idea.

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Advocating process modeling and de-emphasizing parameter estimation

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