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Towards an uncertainty framework for predictions in ungauged basins: The Uncertainty Working Group

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Abstract The reduction of predictive uncertainty is the main objective and the main criterion of success for the Predictions in Ungauged Basins (PUB) initiative of IAHS. Achieving this goal requires that an uncertainty framework is created in which models, data and methods can be evaluated with respect to their impact on predictive uncertainty. Here we provide a first overview of the uncertainty working group, including its main objectives and how we intend to achieve them.

Key words hydrological modelling; predictions in ungauged basins; uncertainty

INTRODUCTION

The overall objective of the Predictions in Ungauged Basins (PUB) initiative of the International Association of Hydrological Sciences (IAHS) is to formulate and implement appropriate science programmes to engage and energize the scientific community in a coordinated and effective manner, and so towards achieving major advances in the capacity to make predictions in ungauged basins (Sivapalan *et al*., 2003; Wagener *et al*., 2004). This objective will be achieved by improving existing and developing new innovative models through interactive learning and diagnostic analysis in an uncertainty framework (Fig. 1). In addition, we need to truly understand the extent of our uncertainties in all aspects of the modelling process in order to better understand and quantify our predictive uncertainties. This will, in time, lead to improved understanding of how well we are able to model the systems under study and therefore the hope is that this will lead to reduced predictive uncertainty. Reduction of predictive uncertainty is thus the declared measure of success of the PUB initiative. It

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is important to recognize that such a reduction will only be effective if new theory/modelling, model evaluation and field monitoring techniques are combined and integrated in an overall learning environment. The PUB problem, of course, extends beyond the prediction of water quantity to include water quality, sediment and ecological variables. The majority of the European waterbodies designated by the Water Framework Directive (WFD) are ungauged, at least with respect to some of the variables of interest for such an integrated catchment management framework. The problem might also be slightly different for many, less developed, countries where only remotely sensed information is available in many locations.

The PUB objective is similar to Klemeš (1986) second and fourth validation tests—transferability of a model to a proxy basin without re-calibration. Few examples of attempts to directly use hydrological models in ungauged basins without any use of parameter calibration can be found in the literature (e.g. Parkin *et al*., 1996; Koren *et al*., 2000; Atkinson, 2001; Duan *et al*., 2001). Results were generally of limited

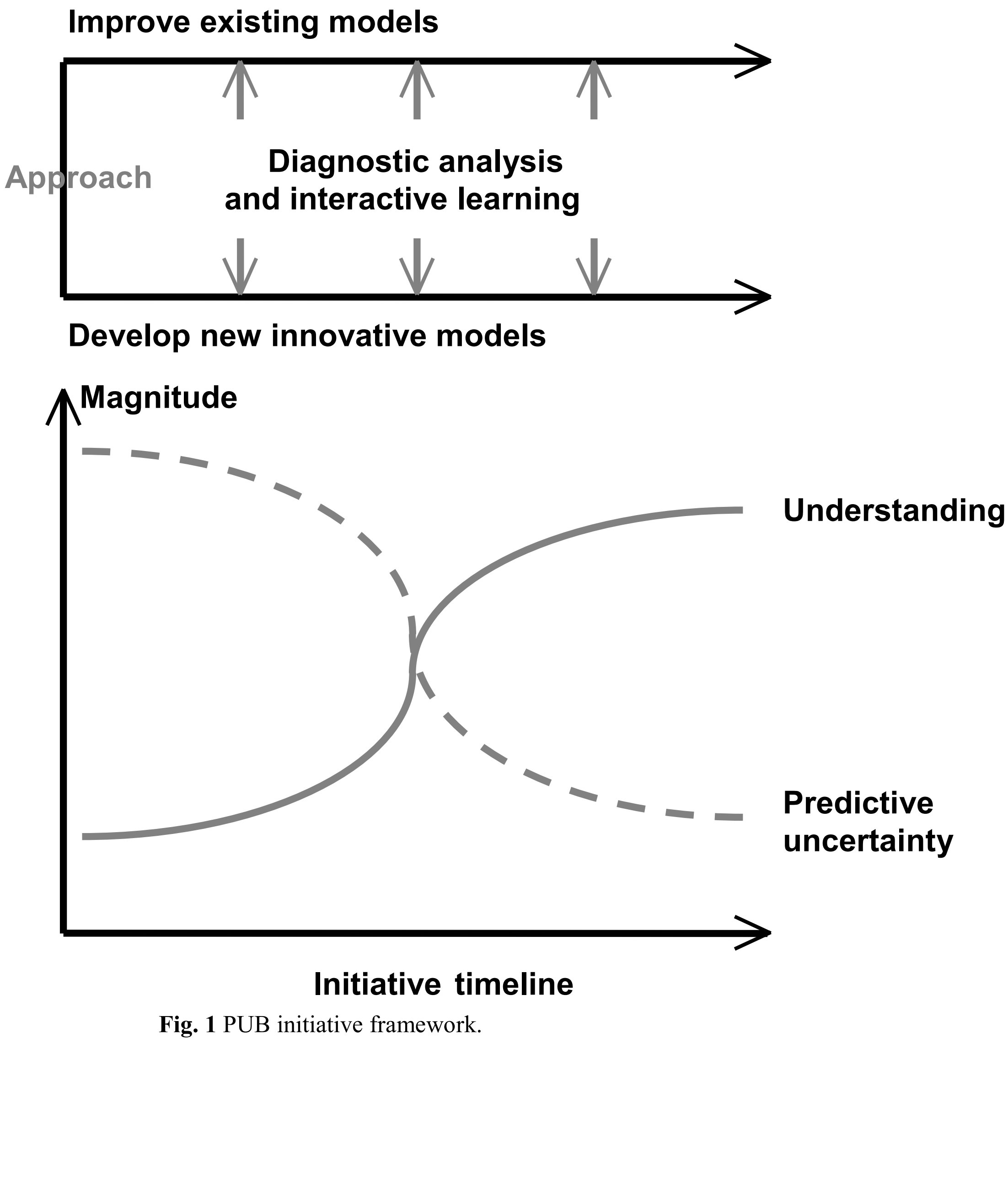

Fig. 1 PUB initiative framework.

success with respect to the reliability of predictions achieved for the ungauged problem and their results have so far been restricted to providing some initial parameter values or ranges for subsequent calibration.

PUB is written in terms of understanding (with subsequent reduction) of uncertainty in the predictive watershed response. Major sources of uncertainty stem from the data; the model (structure and parameters); the perceptual model of the underlying hydrological system; the interplay of inherently incomplete measurements and the nonlinear, sometimes threshold, character of hydrological processes; and the methods used to merge data and models (parameter estimation, etc.). Reductions in predictive uncertainty through improvements in any of these components should therefore to be tested in an uncertainty framework. Such a framework should allow for the consideration of all sources of uncertainty, and be in the form of a diagnostic or learning tool. Important science questions are thus: what is the best strategy to estimate this uncertainty? and What are realistic amounts of uncertainty?

The PUB Working Group (WG) for uncertainty analysis in hydrological modelling has been formed to pursue this question. Its focus lies on analysis of predictive uncertainty through the intelligent consideration of all uncertainties in the modelling process. The WG's main task is *to stimulate progress and give guidance on uncertainty estimation and model diagnostics*.

This paper is an introduction to the uncertainty WG and discusses its set-up, the WG philosophy chosen, and the vehicles that will be used to achieve progress. These initiatives are purposely non-technical in their presentation and so in what follows the focus is on the philosophy and approach chosen by the uncertainty WG.

UNCERTAINTY ESTIMATION

A wide variety of uncertainty estimation methods are available (see recent review by Gupta *et al*., 2005). These approaches vary widely with respect to underlying assumptions, technical implementation, etc. Common to these approaches is the selection or identification of a set (population) of models (different combinations of model structures and parameter values), and an assignment of some relative degree of believability to each member of the set. That degree of believability is translated into interval estimates of the uncertainty (confidence) in model simulations/predictions. The approaches differ in the suite of assumptions underlying each technique, based on how the methods used to compute the relative degree of believability are derived. A list of some of the more popular approaches is provided in Table 1. This list is of course by no means complete and we appreciate that methods are continuously evolving. Despite the differences between the approaches, it is possible to reduce all of them to three basic steps (Beven & Freer, 2001):

(1) What constitutes a behavioural model, i.e. a model that represents an acceptable representation of the system under study?
(2) How do we identify (find) the subset of behavioural models in the feasible model space?
(3) How can we propagate "behavioural predictions" into the output space, while considering the uncertainty in input data and other "model elements"?

Table 1 List of examples of uncertainty methods applied in hydrological modelling.

Name	Main reference
BARE	Thiemann, M., Trosset, M., Gupta, H. V. & Sorooshian, S., (2001) Bayesian recursive parameter estimation for hydrologic models. *Water Resour. Res*. **37**(10), 2521–2536, 10.1029/2000WR900405.
BATEA	Kavetski, D. N., Franks, S. W. & Kuczera, G., (2002) Confronting uncertainty in rainfall–runoff modelling: a global system analysis perspective. In: *Advances in Calibration of Watershed Models* (ed. by Q. Duan *et al.*), 49–68. American Geophysical Union, Washington DC, USA.
BFS	Krzysztofowicz, R. (1999a) Bayesian theory of probabilistic forecasting via deterministic hydrologic model. *Water Resources Res*. **35**, 2739–2750.
BPO / BPE	Krzysztofowicz, R. (1999b) Bayesian forecasting via deterministic model. *Risk Analysis* **19**, 739–749.
DBM	Young, P. (1998) Data-based mechanistic modelling of environmental, ecological, economic and engineering systems. *Environ. Modelling and Software* **13**, 105–122.
DYNIA	Wagener, T., McIntyre, N., Lees, M. J., Wheater, H. S. & Gupta, H. V. (2003) Towards reduced uncertainty in conceptual rainfall-runoff modelling: Dynamic identifiability analysis. *Hydrol. Processes* **17**(2), 455–476.
GLUE	Beven, K. J. & Freer, J. (2001) Equifinality, data assimilation, and uncertainty estimation in mechanistic modelling of complex environmental systems. *J. Hydrol* . **249**, 11–29
GRUE	Beven, K. J. (2005) A manifesto for the equifinality thesis. *J. Hydrol.* (in press).
MACS	Hogue, T. S., Sorooshian, S. Gupta, H. Holz, A. & Braatz, D. (2000) A multi-step automatic calibration scheme for river forecasting models. *J. Hydrometeorol*. **1**, 524–542.
MCAT	Wagener, T., Lees, M. J. & Wheater, H. S. (2001) A toolkit for the development and application of parsimonious hydrological models. In: *Mathematical Modelling of Large Watershed Hydrology* (ed. by V. P. Singh & D. Frevert). Water Resources Publications LLC, USA.
MCMCS	Bates, B. C. & Campbell, E. P. (2001) A Markov chain Monte Carlo scheme for parameter estimation and inference in conceptual rainfall-runoff modelling. *Water Resour. Res*. **37**, 937–947.
META-G	Montanari, A. & Brath, A. (2004) A stochastic approach for assessing the uncertainty of rainfall–runoff simulations. *Water Resour. Res*. **40**, doi:10.1029/2003WR002540.
MLBMA	Neuman, S. P. (2003) Maximum likelihood Bayesian averaging of alternative conceptual-mathematical models. *Stochast. Environ. Res. Risk Assessment* **17**(5), 291–305, 10.1007/s00477-003-0151-7,.
MOCOM-UA	Yapo, P. O., Gupta, H. V. & Sorooshian, S. (1998) Multi-objective global optimization for hydrologic models. *J. Hydrol.* **204**(1–4), 83–97.
MOGSA	Bastidas, L. A., Gupta, H. V., Sorooshian, S., Shuttleworth, W. J. & Yang, Z. L. (1999) Sensitivity analysis of a land surface scheme using multi-criteria methods. *J. Geophys. Res.* **104**, No D16, 19 481–19 490.
Mx Fit	Pappenberger, F. & Beven, K. (2006) Functional classification and evaluation of hydrographs based on multicomponent mapping. *Int. J. River Basin Manage*. (in press)
NLFIT	Kuczera, G. & Parent, E. (1998) Monte Carlo assessment of parameter uncertainty in conceptual catchment models: The Metropolis algorithm. *J. Hydrol*. **211**(1-4), 69–85.
PARASOL	van Griensven A. & Meixner T. (2004) Dealing with unidentifiable sources of uncertainty within environmental models. In: *Proc. Int. Environ. Modelling and Software Society (iEMSs 2004)* (14–17 June 2004, University of Osnabrück, Germany).
PEST	Doherty, J. & Johnston, J. M. (2003) Methodologies for calibration and predictive analysis of a watershed model. *J. Am. Water Resour. Assoc*. **39**(2), 251–265.
PIMLI	Vrugt, J. A., Bouten, W., Gupta, H. V. & Sorooshian, S. (2002) Toward improved identifiability of hydrologic model parameters: The information content of experimental data. *Water Resour. Res*. **38**(12), art. no. 1312, DOI: 10.1029/2001WR001118,.
SCEM-UA	Vrugt, J. A., Gupta, H.V. Bouten, W. & Sorooshian, S. A (2003) Shuffled Complex Evolution Metropolis algorithm for optimization and uncertainty assessment of

	hydrologic model parameters. *Water Resour. Res*. **39**, 1201, doi:10.1029/2002WR001642,.
SODA	(as above)
SOLO	Hsu, K., Gupta, H.V. Gao, X. Sorooshian, S. & Imam, B. (2002) SOLO–An artificial neural network suitable for hydrologic modelling and analysis. *Water Resour. Res.* **38**(12), 1302.
Soft INFO	Seibert, J. & McDonnell, J. J. (2002) On the dialog between experimentalist and modeler in catchment hydrology: use of soft data for multicriteria model calibration. *Water Resour. Res*. **38**(11), 1241, doi:10.1029/2001WR000978.
SUNGLASSES	van Griensven A. & Meixner T. (2004) Dealing with unidentifiable sources of uncertainty within environmental models. In: *Proc. Int. Environ. Modelling and Software Society (iEMSs 2004)* (14–17 June 2004, University of Osnabrück, Germany).
U-CODE	Poeter, E. P. & Hill, M. C. (1998) Documentation of UCODE, a computer code for universal inverse modelling. *US Geological Survey Water-Resources Investigations Report 98–4080*, 122p. http://pubs.water.usgs.gov/wri984080/

One science question therefore has to be, "Should we still be putting more effort in to developing additional methods?" And if yes, then why, and/or how? Alternatively should we be better spending our energy elsewhere, e.g. to improve connections with experimentalists and so to increase our understanding of the observational uncertainties in the data we are trying to predict. Or to learn how different data sources can be used to better discriminate the behaviour of different subsystems and link this to develop and improve submodels iteratively.

There is currently little guidance available to help decide how these three steps of an uncertainty method should be implemented for different cases, e.g. model type used or available data or the problem at hand. This is due to both a lack of understanding about the impact of the assumptions made and to a lack of information about the applicability of different approaches. Understanding and guidance is needed therefore with regard to what approach(es) should be used as a function of:

- Available data.
- Modelling objective, i.e. the variable of interest.
- Model used, e.g. its complexity and cost of execution.
- Basin characteristics, e.g. climatic regime.

Clearly in many cases, guidance, although warranted, will not equate to a single consensus regarding the utility and advantages/disadvantages of individual techniques. What an uncertainty framework should look like depending on these four criteria is unclear and may well remain so until improvements in models/model evaluation/field techniques are realized. Advances in this respect will come from improved understanding about underlying theory and through comparison studies of available approaches using different case studies.

NATURE OF WORKING GROUP & WORKSHOPS

The Uncertainty Working Group

The Uncertainty WG is open to everybody who is interested in the issue of uncertainty in hydrological or environmental modelling (including field experimentalists)—even if some of the activities might be limited by available capacities, especially when dedicated workshops are held. The focus is on understanding (identifying and quantifying) uncertainty through the intelligent analysis of all uncertainties in hydrological modelling and observation. The main WG task—to stimulate progress and give guidance on uncertainty estimation and model diagnostics—will be achieved by addressing two fundamental science questions:

(1) How to (explicitly) estimate and propagate all sources of uncertainty in hydrological modelling?
(2) What is an appropriate framework for (model/method/data) evaluation under uncertainty?

The short term organizational objective of the Uncertainty Working Group is to develop a global uncertainty network with pairs of scientists (combining young and experienced) on every continent to enable widespread dissemination of results from this working group and to allow for a variety of international workshops in which different issues (topics/applications/geographic requirements) guide its content (Fig. 2). These workshops will be organized by changing members of the Uncertainty Working Group. Furthermore we expect much of the information/debate to be developed using web based information to allow easy open access to activities and understanding. We expect to stimulate discussion and debate in formats where multiple points of view are and should be encouraged.

THE MENAGGIO WORKSHOP

The main vehicle to achieve the above stated WG objectives is in the form of workshops that focus on creating/disseminating knowledge through exchange in small group discussion groups. The first WG workshop in June 2004 in Menaggio (Italy) was one of the first workshops purely focusing on uncertainty analysis and enabled 26 international scientists to discuss this issue over a three-day period.

The Menaggio workshop was experimental in its design and much work went into creating a setting in which knowledge would not just be exchanged, but created. The workshop focused on small group discussions and the only talks included were general introduction talks. The presenters of these talks were young(ish!) scientists who were asked to present an overview with respect to a pre-selected topic, instead of purely presenting their own work. Two of those introduction talks would be presented in the morning to provide a framework for the small group discussions (<10 people) who used pre-defined science questions as further guidelines. After a long lunch break—to allow for socializing—posters with individual research results were (briefly) introduced. A common data set and model were distributed prior to the workshop to provide a direct comparison in the discussions. Participants could walk between the posters, which were all up for three days, and discuss particular research in detail. The day would finish with a plenum (round-table) discussion in which one scientist from the small discussion groups would present the five or so main results/questions/-comments from his/her particular discussion in the morning. These were then open for comment by the whole group. The sense of community was increased by having three extensive daily meals together in which discussion and socializing enabled participants to get to know each other better. Presentations and reports on uncertainty analysis techniques developed and presented at the workshop can be found at http://www.es.-lancs.ac.uk/hfdg/uncertainty_workshop/uncert_intro.htm.

The Menaggio workshop format will serve as a model for future Uncertainty Group workshops and hopefully help other WG to develop similarly productive environments. The workshop was build around three main science questions:

(1) What is the current state of the art of uncertainty analysis in environmental and hydrological science and in other relevant fields?
(2) What are the limitations and problems of current methods? What are the bottlenecks that prevent progress?
(3) What are promising directions for progress in uncertainty analysis in environmental and hydrological science?

CONCLUSIONS, INITIAL RESULTS & OUTLOOK

This paper presents the PUB Uncertainty Working Group including its philosophy, set-up and the vehicles for progress in the defined research area. A framework in which the analysis of uncertainty methods can be performed has been outlined, as well as the general objectives of this particular working group. Initial results (conclusions/comments/questions) of the working group—from the Menaggio workshop in 2004—are listed below and show the current thinking on what is required to advance the field of uncertainty analysis in hydrological modelling and what steps have to be taken to achieve progress:

– We need to establish guidance for selecting appropriate uncertainty approaches. How does method selection depend on criteria such as model complexity or modelling objective?
– We need to develop an uncertain "learning"framework. Such a framework should work as a diagnostic tool and guide modellers to improve their structures, rather than simply act as a tool to propagate uncertainty into the output.
– We need to know more about the meaning of and extent of the errors in our observations.
– We need to work with field scientists to collect data that better quantifies this uncertainty (not just analytical but the representational uncertainties in data).
– We need to establish intense dialogue with field experimentalists to learn about new data sources, and especially about subsurface states, for better constraining parameter estimation.
– We should learn from field scientists about hydrological functioning of different landscapes to allow *a priori* discrimination of unrealistic model structures.
– We need to establish the requirements for an uncertainty framework for less developed regions of the world.

Going beyond the current scientific debate on uncertainty analysis, the working group is also concerned with the transfer of results into practical use. Activities in this context will include the development of tools that combine a variety of uncertainty methods (in collaboration with other initiatives, e.g. the Joint Universal Parameter

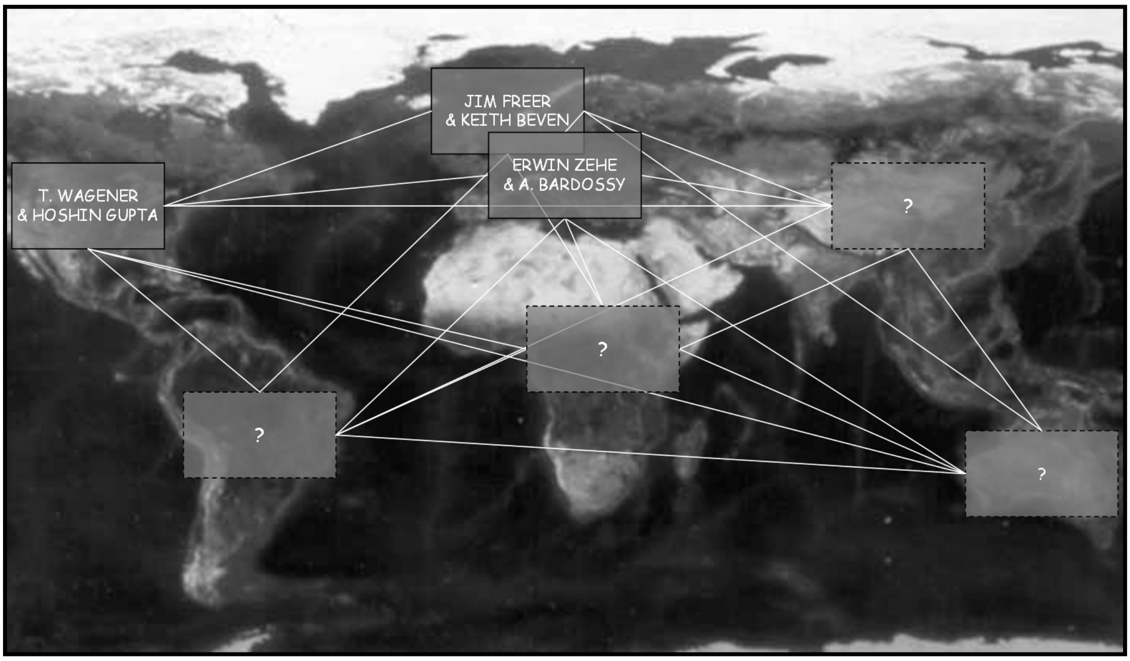

Fig. 2 Towards a global uncertainty network.

IdenTification and Evaluation of Reliability (JUPITER) project [Mary Hill, USGS, personal communication]) and the distribution of different uncertainty analysis codes through globally accessible web-portals (e.g. http://www.sahra.arizona.edu/software). Global connectivity will be attempted through establishing groups of scientists in different geographic areas (Fig. 2) to help with knowledge transfer, particular in less developed countries.

Further information regarding the working group and future activities can be found on the following web-sites: http://www.es.lancs.ac.uk/hfdg/uncertainty_workshop/-uncert_intro.htm and http://www.hwr.arizona.edu/uncertainty/. Available information includes one-page summaries of many popular uncertainty methods and the posters and introduction talks presented at the Menaggio workshop.

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REFERENCES

Atkinson, S. E. (2001) Climate, soil vegetation controls on streamflow variability with changing timescales and implications for model complexity. MSc Thesis, Department of Environmental Engineering, University of Western Australia, Nedlands, Australia (unpublished).

Beven, K. J. & Freer, J. (2001) Equifinality, data assimilation, and uncertainty estimation in mechanistic modelling of complex environmental systems. *J. Hydrol.* **249**, 11–29.

Duan, Q., Schaake, J. & Koren, V. (2001). A priori estimation of land surface model parameters. In: *Land Surface Hydrology, Meteorology, and Climate: Observations and Modelling* (ed. by V. Lakshmi, J. Albertson & J. Schaake). American Geophysical Union, Water Science and Application **3**, 77–94.

Gupta, H. V., Beven, K. J. & Wagener, T. (2005) Model calibration and uncertainty estimation. In *Encyclopedia of*

Hydrological Sciences. (ed. by M. G. Anderson, & J. J. McDonnell). John Wiley & Sons Ltd., Chichester, UK.

Klemes V. (1986) Dilettantism in hydrology: transition or destiny. *Water Resour. Res.* **22**(9), 177–188.

Koren, V. I., Smith, M., Wang, D. & Zhang, Z. (2000) Use of soil property data in the derivation of conceptual rainfall–runoff model parameters. In: *15th Conference on Hydrology* (Long Beach, American Meteorological Society, Paper 2.16, USA).

Parkin, G., O'Donnell, G., Ewen, J., Bathurst, J. C., O'Connell, P. E. & Lavabre, J. (1996) Validation of catchment models for predicting land-use and climate change impacts. 2. Case study for a Mediterranian catchment. *J. Hydrol*. **175**, 595–613.

Sivapalan, M., Takeuchi, K., Franks, S. W., Gupta, V. K., Karambiri, H., Lakshmi, V., Liang, X., McDonnell, J. J., Mendiondo, E. M., O'Connel, P. E., Oki, T., Pomeroy, J. W., Schertzer, D., Uhlenbrook, S. & Zehe, E. (2003) IAHS decade on Predictions of Ungauged Basins (PUB): Shaping an exciting future for the hydrological sciences. *Hydrol. Sci. J.* **48**(6), 857–879.

Wagener, T., Sivapalan, M., McDonnell, J. J., Hooper, R., Lakshmi, V., Liang, X. & Kumar, P. (2004) Predictions in Ungauged Basins (PUB)—A catalyst for multi- disciplinary hydrology. *Eos, Trans. AGU* **85**(44), 451–452.