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Editorial

Towards a new generation of hydrological process models for the meso-scale: an introduction

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1 Focus and background

The main motivation for this special issue of Hydrology and Earth System Sciences is the IAHS decadal research initiative "Predictions in Ungauged Basins" (Sivapalan et al., 2003), and more specifically the need to develop hydrological models that work for the "right reasons" (Kirchner, 2006). This means that a model shall "work" because its structure is based on appropriate representation of the hydrological functioning of a landscape/catchment and the associated dominant patterns and landscape structures, and not because several structural deficits are mutually compensated within the usual model calibration process. The central credo underlying our quest in this direction is that typical patterns of vegetation, soils and subsurface structures within a catchment cause a typical hydrological process spectrum or hydrological functioning represented as a generic feature of a landscape. This is known as the pattern-process-function paradigm in theoretical ecology (Watt, 1947; Turner, 1989; Turner and Gardner; 2001; Schroeder, 2006, this special issue). We, therefore, expect that model structures that offer a higher compatibility with landscape structures and hydrological functioning of catchments will allow, in the long term, much better predictions than may be achieved with currently available conceptual models. The latter type models have the tendency to compensate the model structural error by unrealistic parameter combinations, which are then reflected in large parameter uncertainty (Wagener et al., 2003).

In this light, this special issue presents a series of articles that address the following themes:

- Novel types of meso-scale hydrological process models, advancement of the underlying fundamental concepts, and their application to real world catchments. This, in particular, is with respect to the REW approach (Reggiani et al., 1997, 1998) as well as the Hillslope storage Boussinesq model (HSB, Troch et al., 2003); the concepts behind both modelling approaches are briefly explained below.
- New concepts regarding how to parameterise the effects of subscale structures and heterogeneity within meso-scale process formulations and the related topic of effective material properties. This is the assessment of closure- and constitutive relations and is further discussed in the following sections.
- Promising approaches to partly overcome the "equifinality dilemma" even for current conceptual hydrological models. The essence is to look at model parameter sets as teams, or in combination, instead of as individually independent values.
- How hydrology can benefit from the collaborative research and intellectual exchanges with landscape ecology within a wider earth system context.

Many of the papers that appear in this special issue have been presented earlier during the PUB Symposium held at the IAHS General Assembly in Foz do Iguacu in April 2005. However, the true origins of this special issue go further back to a workshop on "Data Assimilation and Catchment Scale Modelling" held in Wageningen, The Netherlands, in September 2001. It is interesting to note that both the REW approach and the HSB model were already discussed there, however in a controversial manner. It is even more interesting to note that today there are two models based on the REW approach already available and being used operationally: REWASH (Reggiani and Rientjes, 2005; Zhang and Savenije, 2005; Zhang et al., 2006, this special issue) and CREW (Lee et al., 2007, this special issue). And both

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have shown to be applicable to model real world catchments with reasonable success. On the one hand, this is a major step forward. During the workshop in Wageningen the prospect of this happening in less than 10 years was considered highly unrealistic and certainly ambitious. On the other hand, discussions during the review process raised several important objections concerning fundamental assumptions underlying the REW approach. This special issue should be seen as the starting point of a more coherent, open and critical discussion of alternative approaches to the development of hydrological process models for the meso-scale.

In this light the remaining part of this text will provide a framework for the papers appearing in this special issue, highlight the main findings, explain interrelations between different studies, discuss possible contradictions and close with a critical and positive outlook. Since most of the papers deal with the HSB model the REW approach and related research tasks the best start is a short summary of both approaches.

2 The REW approach and related studies

Reggiani et al. (1998, 1999) proposed a novel framework to build meso-scale hydrological models. The heart of the approach is a set of balance equations for mass, momentum and energy that address the dynamics at the scale of a hydrologically significant control volume they named as the Representative Elementary Watershed (REW), which they derived by recourse to volume averaging. To be compatible with the structure of real catchments an REW is subdivided into 5 zones named as: unsaturated zone, saturated zone, concentrated and saturated overland flow zones and channel reach. The REW organization explicitly resolves the natural organization of the overall watershed around the river network, and the 5 sub-regions are meant to capture and "parameterize" the effects of unobserved structure within the REW. Mass, energy and momentum balance for the "different zones" within the REW and the exchanges between the REWs are characterised by a set of coupled ordinary differential equations. However, the mass and momentum fluxes between these zones are generally unknown and are not measured routinely. To render these coupled balance equations "determinate" and numerically tractable it is necessary to derive "closure" relations that characterise mass and momentum exchanges in terms of other known state variables and climate and landscape parameters. In analogy to boundary layer meteorology and fluid mechanics, this derivation procedure has been named "closure" or the "closure problem".

The studies presented in this special issue aim either at

- Advancing the REW theory in a fundamental way and/or applying numerical models based on the REW approach to meso- and micro-scale catchments in different hydro-climates (Tian et al., 2006; Varado et al., 2006; Zhang et al., 2006; Lee et al., 2007, this special issue);
- How to solve the closure problem and how to assess constitutive relations such as effective soil water characteristics, ideally through upscaling without calibration (Lee et al., 2007; Zehe et al., 2006; Beven, 2006, this special issue).

2.1 Advancement of the REW approach and applications of REWASH

In their study entitled "Extension of the Representative Elementary Watershed approach by incorporating energy balance equations" Tian et al. (2006, this special issue) present an extension of the REW theory to cold regions. They introduce a glacier and snow-covered zone to the existing 5 zones, and write down the related mass and energy balance equations to account for snow accumulation, snow melt and glacier melt. This is of course an important conceptual extension of the REW approach that, firstly, requires extension of the constitutive theory, and once complete the resulting model has to be tested within future applications in appropriate "cold" regions. This work is in progress.

Varado et al. (2006, this special issue) present the application of REWASH to the Donga Basin in Africa within their study "Multi-criteria assessment of the Representative Elementary Watershed approach on the Donga catchment (Benin) using a downward approach of model complexity". The main objective was to reproduce discharge and water table dynamics observed in several wells in the 586 km^2 large Donga basin in Benin, which are strongly influenced by the African Monsoon. The authors essentially compared a finer spatial discretisation that represents second order catchments as single REWs with a coarser one starting with third order catchments. The study suggests that the model yields reasonable predictions of daily discharge values (Nash-Sutcliffe efficiencies ranging from 0.21 to 0.6) for a total catchment area larger than 100 km^2, after calibrating effective soil parameters for the unsaturated zone. Interestingly, the finer scale discretisation did not yield a better model performance, even when used with spatially distributed precipitation input estimated with block kriging. The authors concluded that a more complex representation of the unsaturated zone is needed for a better reproduction of water table dynamics observed especially for perched aquifers. Nevertheless, the study demonstrates the potential of REWASH to yield useful predictions for integrated water management.

The study of "Modelling subsurface stormflow with the Representative Elementary Watershed approach: application to the Alzette River Basin" by Zhang et al. (2006, this special issue) marks a major step towards improved process-based modelling of subsurface stormflow at the meso-scale. The authors extend the REW approach by including a macropore domain for describing subsurface stormflow, and reformulated the mass balance equations and closure relations associated with this new process of subsurface stormflow. Flux in the macropore domain is driven by gravity and can have a vertical as well as a lateral component. The extended REWASH model is applied to the 292 km^2 are Alzette river basin in Luxembourg, where subsurface flow makes a significant contribution to runoff generation. Model parameters are obtained through manual calibration. The model simulations yielded a good match of daily discharge observed at several stations, as well as a reasonable match of groundwater levels observed also at multiple locations. This study shows clearly that REWASH has the potential to reproduce several hydrological signatures in a catchment and to incorporate key processes such as subsurface storm flow.

2.2 The REW approach and the closure problem

We now present three papers that deal fundamentally with the derivation and assessment of closure relations in catchment hydrological modelling. Closure and the derivation of closure relations are relatively new to catchment hydrology, but are much more common in sister disciplines such as fluid mechanics, limnology, atmospheric sciences etc. Even as late as 2001, the most definitive monograph ever published on rainfall-runoff modelling (Beven, 2001) did not mention anything even remotely resembling the issue of closure relations. Part of the reason for this was that a rigorous thermodynamic formalism or theoretical framework did not exist for modelling at the catchment scale until the REW approach was introduced by Reggiani et al. (1998, 1999), who of course explicitly highlighted the issue of closure in respect of the balance equations they had derived at the REW scale. It is therefore interesting, indeed very welcome and timely, that Beven (2006, this special issue) himself has suggested that finding closure relations is no less than the “holy grail” of hydrology.

Development of closure relations at the REW scale is, however, a most difficult task. They are required, first and foremost, to close a set of balance equations, which without them will be indeterminate. In this sense, closure relations automatically imply the existence of an otherwise indeterminate set of balance equations. In the case of the REW approach, the balance equations are explicitly available and closure makes perfect sense. In most other cases, it is only implicit, which is part of the explanation for why hydrologists have not explicitly invoked closure in previous modelling studies. On the other hand, closure relations are also meant to bridge scales – they account for the effects of sub-catchment or sub-REW scale heterogeneities on the exchange fluxes at the catchment or REW scale. How the small scale heterogeneities manifest themselves at the catchment or REW scale, including any change of dominant processes with change of scales, remains a largely unsolved problem, although this is receiving a lot of attention at the present time. How should the closure relations be derived, from below, through integration of models based on small scale theories, or from above, through observations and their interpretations directly at the larger scale? There are competing/complementary approaches suggested:

1. Starting from small scale models that embed the typical hillslope scale heterogeneities for a well observed catchment of interest in them, and then d eriving possible closure relations by averaging the fluxes and states from carefully constructed numerical experiments;

2. Deriving closure relations from carefully designed field experiments that measure the appropriate state variables and fluxes.

The first approach suffers from relying too much on small scale process descriptions and more seriously from the lack of proper approaches to characterise and represent spatial patterns –especially their interactions and connectivity within distributed models. Thus, it might not be able to discover the emergent properties we are actually seeking. The second approach suffers simply from the fact that currently we cannot access the necessary data, especially on subsurface flow dynamics, at the larger control volumes of interest. Furthermore, we do not have the theoretical framework to generalise and extrapolate any relations extracted from these observations to ungauged and unmapped catchments. Clearly, a combination of these two approaches is absolutely essential, i.e. field experiments guided by insights or hypotheses about possible emergent properties and associated closure relations that could potentially be generated within the computer by detailed numerical models.

The three papers in this special issue (Beven, 2006; Zehe et al., 2006; Lee et al., 2007, this special issue) highlight alternative approaches to the derivation of closure relations, and taken together, provide a window into the complexity and difficulty of both approaches.

The paper by Lee et al. (2007, this special issue) entitled “Predictions of rainfall-runoff response and soil moisture dynamics in a microscale catchment using the CREW model” is focused on the derivation of closure relations and effective REW scale material properties using analytical and numerical upscaling methods. The foundation of the numerical upscaling was the highly distributed, well tested, numerical model (CATFLOW) that has been previously demonstrated to reasonably represent the actual land use patterns as well as the typical patterns of soil types and macropores within the Weiherbach catchment in Germany. Lee et al. (2007, this special issue) used the CATFLOW model, through carefully designed numerical (infiltration and drainage) experiments conducted as if the model behaviour (including internal dynamics and overall catchment responses) are a best estimate of reality, for deriving closure relations for seepage flow and geometric relations for variable contributing area, both as functions of saturated storage. A number of other closure relations for a number of other exchange fluxes, such as infiltration and evapotranspiration, were derived separately using analytical averaging of the corresponding point scale equations. Finally, Lee et al. employed time series of the catchment scale average unsaturated hydraulic conductivity, soil saturation and suction obtained during a one year simulation of the catchment scale water balance for estimating effective REW scale average hydraulic properties for the for the unsaturated zone. Lee et al. (2007, this special issue) then incorporated the so-derived closure relations into the coupled REW scale mass and momentum balance equations and on the basis of these developed a distributed REW scale numerical model named CREW. Sensitivity tests and an application of CREW to simulate the catchment scale water balance in the Weiherbach demonstrated that most of the derived closure relations and the related parameters values were feasible without further parameter tuning. However, this was not the case for the effective REW scale hydraulic properties of the unsaturated zone: the functional form turned out to be useful whereas the parameters had to be recalibrated to match the observed rainfall runoff behaviour.

The companion paper by Zehe et al. (2006, this special issue) entitled "Dynamical process upscaling for deriving catchment scale state variables and constitutive relations for meso-scale process models" is almost exclusively focused on the derivation of effective REW scale hydraulic properties. Their approach is a refinement of what was used in 7, this issue). Similar to Lee et al., they too employed the physically based distributed model, CATFLOW, which represents well the hillslope scale patterns and structures in the Weiherbach catchment, to simulate numerical drainage and wetting experiments. In contrast, Lee et al. used the full catchment scale model, driven by natural boundary conditions (rainfall, ET), and obtained spatially averaged soil saturation, matric head as well as the unsaturated hydraulic conductivity at each time step over the entire catchment volume, and estimated effective REW scale hydraulic properties (and closure relations) from these. Zehe et al. (2006, this special issue) used a single typical hillslope and performed drainage and wetting experiments separately using artificial boundary conditions, which gave them a wide range of soil moisture dynamics. For deriving effective REW scale relationships for unsaturated hydraulic conductivity they used, regardless of the point-scale hydraulic conductivity values that evolved in time inside the domain, the averaged in/outflows at the lower boundary of the domain, the average values of soil saturation, and combined these with the theoretical expression for the REW-scale recharge velocity derived by Regginai et al. (1999). The parameters of the effective REW scale hydraulic properties derived through this up-scaling procedure turned out to be close to those that Lee et al. (2006, this special issue) obtained through manual calibration. Zehe et al. (2006, this special issue) showed furthermore that hysteresis of the effective REW scale soil water characteristics in the Weiherbach catchment is small, and may be neglected as a first approximation. This provides an explanation for why Zhang et al. (2006, this special issue), Varado et al. (2006, this special issue) and Lee et al. (2007, this special issue) found a non-hysteretic formulations for effective REW scale soil water characteristics to be sufficient within their applications.

Beven (2006, this special issue) in his paper "Searching for the holy grail of scientific hydrology as closure", explains that finding the solution to the closure problem would be the defining act of scientific hydrology, effectively its "holy grail". Beven suggests that the closure problem indeed exists in every hydrological model, and in every water quality or sediment transport model. In a departure from the work of Lee et al. (2007, this special issue) and Zehe et al. (2006, this special issue), Beven argues that the REW approach, being a control volume representation, will not be consistent with continuum mechanics representations at any useful scale due to the interactions between nonlinearities and heterogeneities in the system. Indeed, due to multiple pathways and residence times in the system, these may not necessarily lead to simple functional relationships between average storages or average gradients of potential and the boundary fluxes, as in the case of most upscaling approaches. An obvious example of this is hysteresis, which exists at all scales, which, Beven argues, is an indication of the failure of the continuum representation. For these reasons, Beven has strenuously argued in his paper, as well as in his discussion of the papers by Lee et al. and Zehe et al. that averaging or upscaling based on small scale distributed descriptions to represent the integrated fluxes at the REW scale will be found to be wholly inadequate. He thus calls for the effects of variability in properties, gradients and divergences at the sub-REW scale to be parameterized or represented directly at the scale of the REW. In conclusion, Beven argues for the use of a very wide range of choices of conceptual parameterisations as multiple competing hypotheses for the closure problem (presumably, the upscaled results being one of them!), which can be tested by taking certain critical measurements.

3 Hillslope storage Boussinesq model and related studies

The Hillslope storage Boussinesq model (HSB, Troch et al., 2003) is based on an analytical solution of the linearised Boussinesq equation that describes discharge from a free unconfined aquifer that develops over impermeable bedrock. The HSB model is tailored for hilly landscapes with shallow, permeable, weakly heterogeneous soils, where subsurface stormflow and saturation excess overland flow dominate runoff generation. Recent studies by Berne et al. (2005) suggest that geomorphic controls on hillslope runoff response and runoff recession maybe characterized by the hillslope Peclet number that relates the product of slope length and average slope to the average depth of the aquifer multiplied by a hillslope width function that distinguishes between convergent, parallel and divergent hillslope. However, to advance the HSB into a model that is applicable to real world catchments, a number of problems have to be solved:

- How to include the effect of the unsaturated zone and soil heterogeneity within the analytical approach?
- How to derive the necessary parameters, especially the width functions for real catchments?

The paper entitled "Curvature distribution within hillslopes and catchments and its effect on the hydrological response" by Bogaart and Troch (2006, this special issue) addresses the second point. It presents a new algorithm for deriving hillslope width functions from flow length distribution for the example of the Plynlimon catchments in Wales. The most interesting finding is that the majority of the grid cells in this catchment have negative contour curvatures, which suggest overall divergent catchment behaviour. The authors demonstrate that the essential catchment feature to generate flow that "globally" converges to the catchment outlet is controlled by extreme values of DEM grid cells that have entirely a positive curvature and belong to the grid cells in the channel reach. A final numerical experiment shows that the HSB is able to account for the newly derived morphological characteristics and quantify the effects on storage an runoff generation. This is, without doubt, a step forward in the development of a new generation of models that are based on hillslopes as building blocks.

4 Studies on important perspectives for hydrology

We finally present two studies that are both related to mesoscale modelling and offer important perspectives without referring to the REW approach or the HSB model.

One is dealing with the "equifinality dilemma". Bárdossy (2007, this special issue) suggests in his study entitled "Calibration of hydrological model parameters for ungauged basins", that equifinality is less dramatic than is usually suggested by looking at dotty plots. The essence is to look at acceptable model parameter sets as vectors of inter-related parameters, where changes of single parameter values are compensated by changes of related parameters. This is illustrated by the application of the Nash cascade model to the Kocher catchment in Germany. Dotty plots of acceptable parameters look as usual, and indicate a high degree of uncertainty. However, in the two-dimensional parameter space acceptable parameter vectors are located along a hyperbolic curve. Thus, if we select a distinct value of parameter k there is only a limited range of n values that form together as an optimal parameter set. The Hausdorff dimension of this manifold is slightly larger than 1 and not 2. This suggests that catchment response, in this case average lag time of the Nash cascade, is much less uncertain than is suggested by parameter uncertainty. Also for the HBV model applied to two subcatchments of the Neckar basin, the author shows further that the Hausdorff dimension of the manifold of acceptable parameters is much smaller than the linear dimension of the parameter spaces (which was 5). He shows furthermore, that the fact that values of different parameters in a model parameter vector interact and compensate in fact facilitates the transfer of model parameter sets between catchments, provided that suitable constraints are introduced. Overall, the paper suggests that the partly strong interdependence of hydrological parameter in a parameter set my help to overcome the equifinality problem and over-parameterisation of hydrological models.

The paper by Schrder (2006, this special issue) on "Pattern process and function in landscape ecology and catchment hydrology –how can quantitative landscape ecology support predictions in ungauged basins" deals with the so-called "ecological perspective". The author gives convincing evidence from the literature and his own work that the concepts of "pattern, process and function" have been developed coherently within (eco-) hydrology and landscape ecology. He suggests that these common concepts provide guidance for linking research in landscape ecology and in hydrology in a wider geo-ecosystem context. In this sense, one discipline acts as an auxiliary discipline for the other, as illustrated by different examples taken from riverine and semi-arid landscapes. More visionary is the idea to develop coupled models that employ the concept of functional groups of species in ecology and the complementary idea of functional units in hydrology.

5 Closing remarks and future perspectives

This is a relatively small special issue that focuses on a new generation of modelling approaches at the meso-scale that are able to explicitly resolve observed structure at the watershed scale, especially the network structure, and then parameterize the effects of the remaining unobserved or unobservable structure on mass and momentum exchange fluxes at the larger scale. The REW approach was highlighted in this special issue in a major way, with a number of examples of its application for the development of a new generation of distributed models at the watershed scale. A fundamental issue that has been highlighted and debated is the derivation of closure relations, which has been raised to the level of the second most important scientific priority in the paper by Beven (2006, this special issue). This is an important development, in the light of new initiatives such as the predictions of ungauged basins (PUB) initiative, and the push for the setting up of large scale hydrologic observatories in the USA.

What we have learned during the on-line discussion of the REW application and closure papers is that there is still considerable uncertainty about essential fundamentals in REW theory and the closure problem. Can we employ continuum approaches for describing average dynamics at the sub-REW scale? What about the “R” part of the REW, i.e. representativeness? Is the REW the means to separate spatial scales in the sense that the minimum extend of an REW is the ergodic length scale? This question was discussed in some detail. However, another very important question that goes to the foundation of the REW approach has only been discussed in passing. Can we assume local equilibrium at the REW scale? This is a pre-requisite for assuming that effective REW scale state variables in the unsaturated zone are reasonable macroscopic representations of the “microscopic” sub-REW distributions of the moisture state. It is clear that this assumption becomes more and more problematic with the increasing size of REW in the lateral direction and with increasing depth of the unsaturated zone. Hence, the assumptions of ergodicity and of local equilibrium are coincident conditions, with the additional problem that fulfilling one could mean to violation of the other. Allowing a vertically distributed representation of the unsaturated zone could help overcome the problem but at the same time unravel some of the benefits of the REW approach: future research should explore revision of the REW approach to address this problem.

Concerning closure, we believe that research on the effects of sub-REW heterogeneities is already moving beyond mere averaging of small scale process descriptions and associated effective properties, and towards deriving large scale manifestations of the heterogeneities such as connectivity, nonlinear storage-discharge relations, and connecting them to structure and function. Of course, much less work is being done in the field, via field experiments. We hope that raising the interest in “closure relations” in this kind of forum will provide more of the motivation needed to embark on more focused and theoretically guided field studies. On the other hand, hydrologic modelling cannot wait for the many years and even decades that it will take for these closure relations to reach the level of maturity that is consistent with our requirements. The REW approach and the HSB approach must proceed, using closure relations that are already around, or are derived in a way as introduced here, linking the REW scale responses to parameters that describe landscape structure at the REW and sub-REW scales (soils, topography, vegetation) as well as currently possible. Only then can we learn from these experiences and the associated shortcomings to sharpen our research questions for the next research iteration.

To summarize, we have to become much clearer about the meaning of our theories in future discussions; this special issue has been a catalyst towards accelerating this discussion process. A most fruitful development is that scientists from soil physics have become involved in the discussions, and raised the important issue about the local equilibrium and whether a zero dimensional unsaturated zone is sufficient for modelling the hydrological functioning of unsaturated zone soils. This shows again that we have to be ready to critically evaluate and modify the foundations of the REW (or any other) theory. But it also shows that a focus on closure relations has the potential to stimulate knowledge transfer from closely related, more fundamental disciplines such as soil physics and fluid mechanics. Similarly, the paper by Schröder (2006, this special issue) reviewed the concepts of pattern, process and function in landscape ecology, and explored whether the REW can be deemed a “functional unit” in the hydrological sense and whether the concepts of landscape ecology can then help support hydrologic predictions. There is no question that hydrology and hydrologic predictions can benefit from the interactions with soil physics, fluid mechanics and landscape ecology. The REW approach through its focus on numerical modelling and the unknown closure relations does indeed provide – despite its short comings the best theoretical framework for improved predictions as well as fundamental scientific breakthroughs.

We do hope that the papers appearing in this special issue will provide the motivation to other scientists around the world who are thinking along similar lines to join forces and address these twin problems – to advance the development of closure relations, and to work with what we have now to advance hydrological predictions in the best way we can – in a spirit of cooperation within the hydrological community and across the interfaces with neighbouring disciplines.

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